

10/521,531

07/16/2008

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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 8.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPCI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAPLUS and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	22	APR 28	IMSRESEARCH reloaded with enhancements
NEWS	23	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS	24	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	25	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	26	JUN 06	KOREAPAT updated with 41,000 documents
NEWS	27	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS	28	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS	29	JUN 25	CA/CAPLUS and USPAT databases updated with IPC reclassification data

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07/16/2008

NEWS 30 JUN 30 AEROSPACE enhanced with more than 1 million U.S.  
patent records  
NEWS 31 JUN 30 EMBASE, EMBAL, and LEMBASE updated with additional  
options to display authors and affiliated  
organizations  
NEWS 32 JUN 30 STN on the Web enhanced with new STN AnaVist  
Assistant and BLAST plug-in  
NEWS 33 JUN 30 STN AnaVist enhanced with database content from EPFULL

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,  
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that  
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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 09:51:25 ON 16 JUL 2008

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:51:49 ON 16 JUL 2008  
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STRUCTURE FILE UPDATES: 15 JUL 2008 HIGHEST RN 1034171-01-1  
DICTIONARY FILE UPDATES: 15 JUL 2008 HIGHEST RN 1034171-01-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

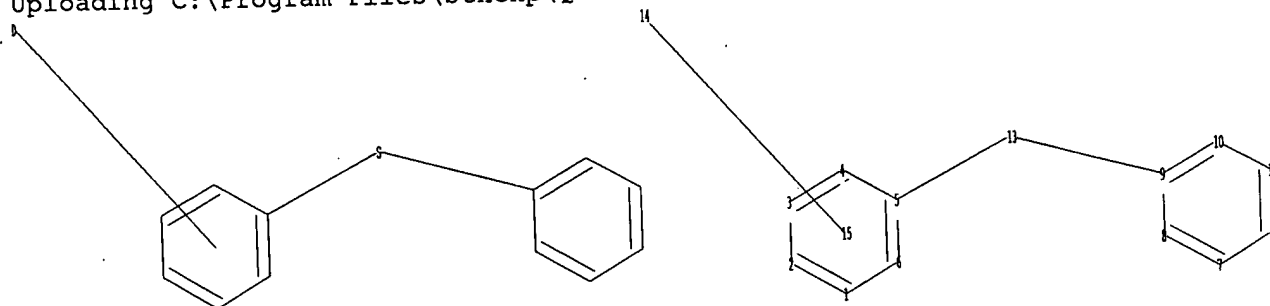
Please note that search-term pricing does apply when  
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=&gt;

Uploading C:\Program Files\Stnexp\Queries\dd3.str.



chain nodes :

13 14

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

5-13 9-13

ring bonds :.

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

5-13 9-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

Match level :

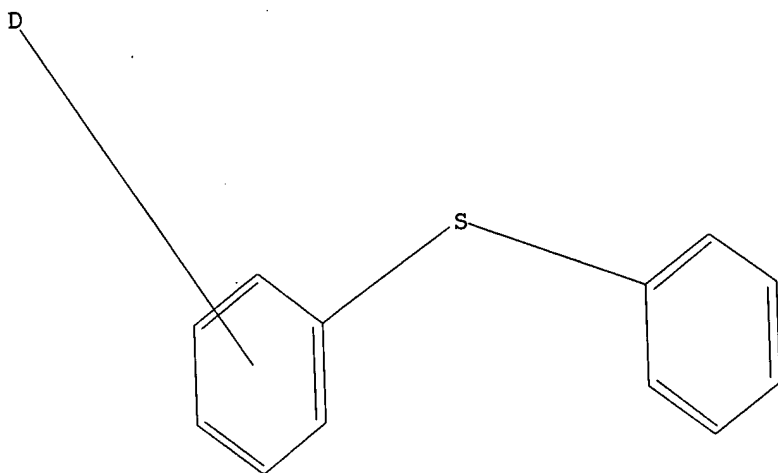
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:CLASS 14:CLASS 15:Atom

L1 STRUCTURE UPLOADED

=&gt; d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 09:52:18 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 257915 TO ITERATE

100.0% PROCESSED 257915 ITERATIONS  
SEARCH TIME: 00.00.01

79 ANSWERS

L2 79 SEA SSS FUL L1

=> file caplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
178.36	178.57

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 09:52:32 ON 16 JUL 2008  
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FILE COVERS 1907 - 16 Jul 2008 VOL 149 ISS 3  
FILE LAST UPDATED: 15 Jul 2008 (20080715/ED)

Caplus now includes complete International Patent Classification (IPC)

reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.  
They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> s 12

L3 46 L2

=> d 13 ibib abs hitstr 1-46

L3 ANSWER 1 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:231432 CAPLUS

DOCUMENT NUMBER: 148:426377

TITLE: Determination of the absolute configurations of isotopically chiral molecules using vibrational circular dichroism (VCD) spectroscopy: the isotopically chiral sulfoxide, perdeuteriophenyl-phenyl-sulfoxide

AUTHOR(S): Drabowicz, Jozef; Zajac, Adrian; Lyzwa, Piotr; Stephens, Philip J.; Pan, Jian-Jung; Devlin, Frank J.

CORPORATE SOURCE: Centre of Molecular and Macromolecular Studies, Department of Heteroorganic Chemistry, Polish Academy of Sciences, Lodz, 90-363, Pol.

SOURCE: Tetrahedron: Asymmetry (2008), 19(3), 288-294

CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The (+) and (-) enantiomers of the isotopically chiral sulfoxide, perdeuteriophenyl-phenyl-sulfoxide, 1, have been synthesized by the reaction of the diastereomers of O-menthyl benzenesulfinate with C6D5MgBr. Their absolute configurations have been determined by comparison of the vibrational

CD (VCD) spectra of (R)-1 and (S)-1, predicted using ab initio DFT, to the exptl. VCD spectrum of 1. The absolute configuration of 1 is shown to be (S)(+)/(R)(-). This is the first application of VCD to the determination of the

absolute configuration of an isotopically chiral sulfoxide.

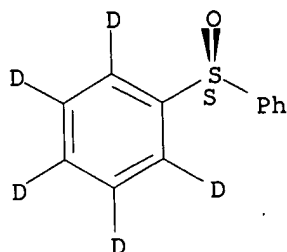
IT 1017265-33-6P 1017265-34-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(absolute configurations of isotopically chiral mols. using vibrational CD (VCD) spectroscopy: isotopically chiral sulfoxide, perdeuteriophenyl-phenyl-sulfoxide)

RN 1017265-33-6 CAPLUS

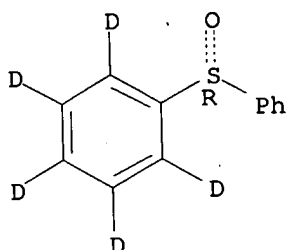
CN Benzene-1,2,3,4,5-d5, 6-[(S)-phenylsulfinyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 1017265-34-7 CAPLUS  
 CN Benzene-1,2,3,4,5-d5, 6-[(R)-phenylsulfinyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:1437488 CAPLUS  
 DOCUMENT NUMBER: 148:215422  
 TITLE: Cyclic and multicyclic poly(ether sulfone)s by polycondensation of 5,5',6,6'-tetrahydroxy-3,3,3',3'-tetramethyl spirobisindane and 4,4'-difluorodiphenylsulfone  
 AUTHOR(S): Kricheldorf, Hans R.; Bornhorst, Kirstin  
 CORPORATE SOURCE: Institut fuer Technische und Makromolekulare Chemie der Universitaet Hamburg, Hamburg, D-20146, Germany  
 SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry (2007), 45(23), 5597-5605  
 CODEN: JPACEC; ISSN: 0887-624X  
 PUBLISHER: John Wiley & Sons, Inc.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB 5.5',6,6'-Tetrahydroxy-3,3,3',3'-tetramethyl spirobisindane (TTSBI) was polycondensed with 4,4'-difluorodiphenylsulfone (DFDPS) in DMSO with K<sub>2</sub>CO<sub>3</sub> as catalyst and azeotropic removal of water. The feed ratio of DFDPS/TTSBI was varied from 1.0/1.0 to 2.0/1.0 at concns. avoiding gelation. At feed ratios around 1.0/1.0 hyperbranched polymers were a minority and cyclic poly(ether sulfone)s were the predominant reaction products. With increasing feed ratio of DFDPS more and more multicyclic polymers were formed, and at a feed ratio of 1.9/1.0 perfect multicycles free of functional groups were the vast majority of the reaction product. Despite variation of the reaction conditions quant. conversion was not achieved.  
 IT 1004993-75-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(cyclic and multicyclic poly(ether sulfone)s by polycondensation of  
tetrahydroxytetramethyl spirobisindane and difluorodiphenylsulfone)

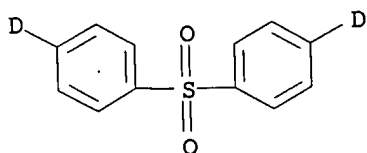
RN 1004993-75-2 CAPLUS

CN 1,1'-Spirobi[1H-indene]-5,5',6,6'-tetrol, 2,2',3,3'-tetrahydro-3,3,3',3'-  
tetramethyl-, polymer with 4,4'-sulfonylbis[benzene-d] (CA INDEX NAME)

CM 1

CRN 1004993-74-1

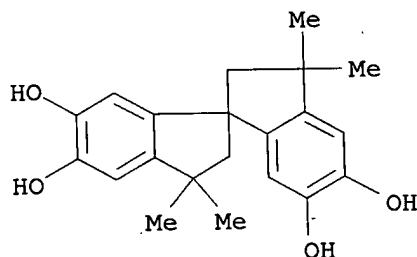
CMF C12 H8 D2 O2 S



CM 2

CRN 77-08-7

CMF C21 H24 O4



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2007:1003746 CAPLUS  
DOCUMENT NUMBER: 148:585487  
TITLE: Synthesis of 13C6, 3H, and 14C labeled Sch 414319 and  
35S labeling of an analog, Sch 225336  
AUTHOR(S): Lavey, Carolee Flader; Hesk, David; Hendershot,  
Sharon; Koharski, David; Saluja, Surinderjit;  
McNamara, Paul  
CORPORATE SOURCE: Schering-Plough Research Institute, Kenilworth, NJ,  
07033, USA  
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals  
(2007), 50(5-6), 264-272  
CODEN: JLCRD4; ISSN: 0362-4803  
PUBLISHER: John Wiley & Sons Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Carbon-, tritium- and sulfur-labeled aryl o-phenylenedisulfones Sch 414319

(1) and Sch 225336 (2), cannabinoid inverse agonists, were prepared. Compds. 1 and 2 are cannabinoid inverse agonist with potential application for the treatment of psoriasis, multiple sclerosis, and rheumatoid arthritis. Three labeled forms, 1-T6, 1-13C6 1-14C were prepared for use as a standard in

a mass spectrometry-based bioanal. assay and to assess metabolism, resp. The 35S-labeled mesylated analog 2 was prepared to study the binding kinetics of the CB2 receptor.

IT 1028184-39-5P 1028184-40-8P 1028184-41-9P

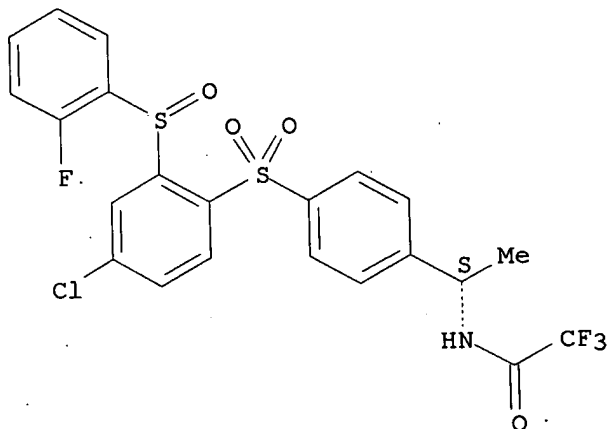
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aromatic o-phenylenedisulfone cannabinoid inverse agonists labeled with carbon and sulfur isotopes and tritium)

RN 1028184-39-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

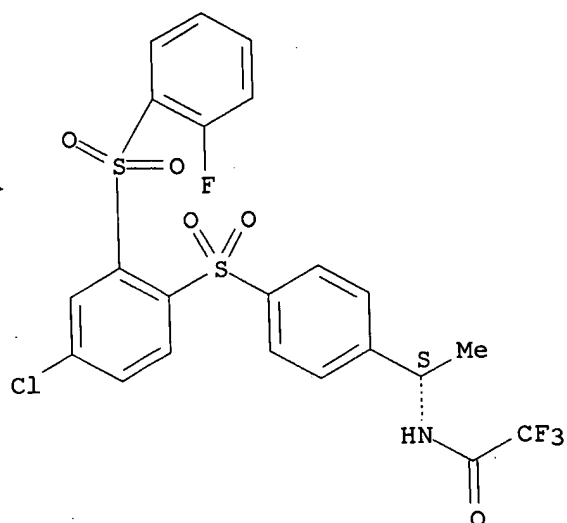


RN 1028184-40-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

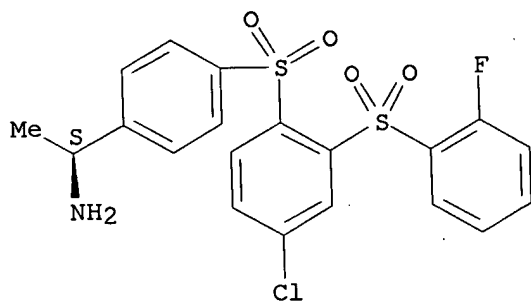
Absolute stereochemistry.





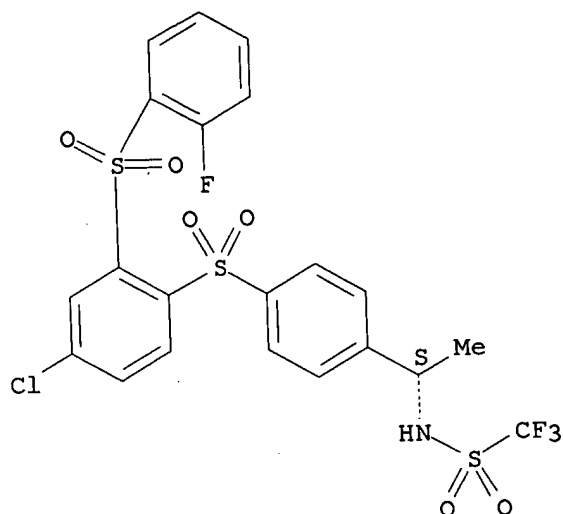
RN 1028184-41-9 CAPLUS  
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



IT 1028184-43-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of aromatic o-phenylenedisulfone cannabinoid inverse agonists  
labeled with carbon and sulfur isotopes and tritium)  
RN 1028184-43-1 CAPLUS  
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:205640 CAPLUS

DOCUMENT NUMBER: 145:433962

TITLE: Quantification of 11C-MADAM binding to the serotonin transporter in the human brain

AUTHOR(S): Lundberg, Johan; Odano, Ikuo; Olsson, Hans; Halldin, Christer; Farde, Lars

CORPORATE SOURCE: Department of Clinical Neuroscience, Section of Psychiatry, Karolinska Institutet, Stockholm, Swed.

SOURCE: Journal of Nuclear Medicine (2005), 46(9), 1505-1515  
CODEN: JNMEAQ; ISSN: 0161-5505

PUBLISHER: Society of Nuclear Medicine

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 11C-N,N-Dimethyl-2-(2-amino-4-methylphenylthio)benzylamine (11C-MADAM) is a newly synthesized radioligand with high selectivity and specificity for the serotonin transporter (5-HTT) in a monkey model. The purpose of this study in humans was to examine the suitability and potential of 11C-MADAM for quant. PET studies of 5-HTT in applied clin. studies on the pathophysiol. and treatment of neuropsychiatric disorders. Methods: PET examination was performed on each of 9 male subjects after i.v. injection of 11C-MADAM with high specific radioactivity. Radioactive metabolites in plasma were determined with high-performance liquid chromatog. A metabolite-corrected

arterial input function was used in kinetic 2- and 3-compartment analyses. Cerebellum was used as the reference region in a cross-validation of 6

reference tissue approaches. Results: The highest radioactivity concentration was detected

in the raphe nuclei, followed consecutively by the striatum, hippocampal complex, cingulate cortex, neocortex, and cerebellum. The time-activity curve for the fraction of unchanged 11C-MADAM in plasma was best described by a sigmoid function. After 50 min, the fraction was 40%. The labeled metabolites were more polar than the mother compound The compartment model

approaches converged, and could describe the time-activity curves in all regions. The total volume of distribution (Vt) was similar to the regional distribution vols. obtained by the linear graphic anal. The binding potentials (BPs) for 6 different approaches yielded similar values in all regions but the raphe nuclei, where the 2 equilibrium methods provided lower values. Conclusion: The regional binding distribution of 11C-MADAM is consistent with postmortem data acquired with 3H-MADAM as well as with that of other reference ligands in vitro. The time-activity curves were well described by current major quant. approaches. The suitability of the cerebellum as a reference region for nonspecific 11C-MADAM binding could be confirmed, thus paving the way for exptl. less demanding approaches, such as the simplified reference tissue model, for applied clin. studies.

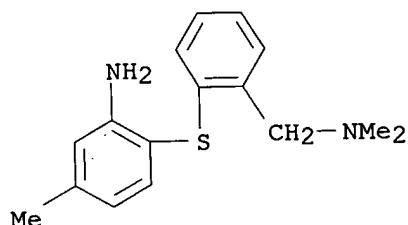
IT 912931-76-1

RL: DGN (Diagnostic use); PKT (Pharmacokinetics); BIOL (Biological study);  
USES (Uses)

(PET ligand 11C-MADAM binding to serotonin transporter in human brain)

RN 912931-76-1 CAPLUS

CN Benzenemethanamine, 2-[(2-amino-4-methylphenyl)thio]-N,N-dimethyl-,  
labeled with carbon-11 (9CI) (CA INDEX NAME)



REFERENCE COUNT:

39

THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1262523 CAPLUS

DOCUMENT NUMBER: 144:23540

TITLE: High refractive index deuterated polyimides and  
derivatives with good transparency, low moisture  
absorption and optical transmission losses, heat  
resistance, and adhesion

INVENTOR(S):

Muto, Kazushige; Maesawa, Tsuneaki; Ito, Nobuhiro;  
Watahiki, Tsutomu; Hirota, Kosaku; Sajiki, Hironao

PATENT ASSIGNEE(S):

Wako Pure Chemical Industries, Ltd., Japan

SOURCE:

PCT Int. Appl., 71 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

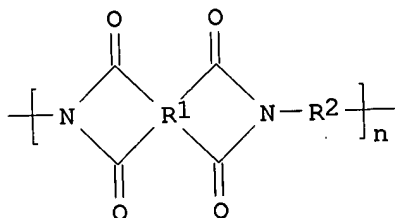
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,  
 SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,  
 ZA, ZM, ZW  
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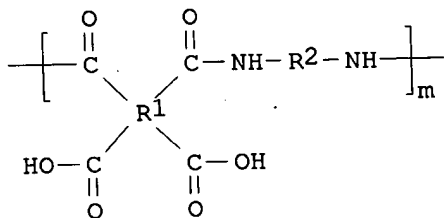
CA 2567487 A1 20051201 CA 2005-2567487 20050517  
 EP 1754739 A1 20070221 EP 2005-741155 20050517  
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 IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR  
 CN 1957019 A 20070502 CN 2005-80016299 20050517  
 US 20080045724 A1 20080221 US 2006-569463 20061121  
 JP 2004-151209 A 20040521  
 WO 2005-JP8984 W 20050517

PRIORITY APPLN. INFO.:

GI



I



II

AB Title polyimides useful as the raw material of polymers for optical waveguides have a deuterated structure I obtained by ring-closure reaction of deuterated polyamic acid II produced by reacting an optionally deuterated acid anhydride with a deuterated diamine, wherein R1 = tetravalent alicyclic or aromatic hydrocarbon group which may be deuterated; and R2 = deuterated divalent aromatic hydrocarbon group; and m, n =  $\geq 1$  integer. Thus, 20 g o-tolidine and 680 mL D2O were reacted in the presence of 2 g 10% Pd/C and 4 g 5% Pt/C at 80° for 24 h, 10 mmol of which was polymerized with 10 mmol pyromellitic anhydride at 25° for 2 h to give a deuterated polyamic acid with eight average mol. weight 168,000, 10% solution of the resulting copolymer was cast onto a glass, heated at 200° for 1 h and 300° for 1 h to give a deuterated polyimide.

IT 870284-75-6P

RL: IMF (Industrial manufacture); RCT (Reactant); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(high refractive index deuterated polyimides and derivs. with good transparency, low moisture absorption and optical transmission losses, heat resistance, and adhesion)

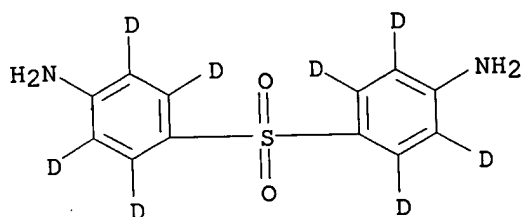
RN 870284-75-6 CAPLUS

CN 1H,3H-Benzo[1,2-c:4,5-c']difuran-1,3,5,7-tetrone, polymer with 4,4'-sulfonylbis[benzen-2,3,5,6-d4-amine] (9CI) (CA INDEX NAME)

CM 1

CRN 557794-38-4

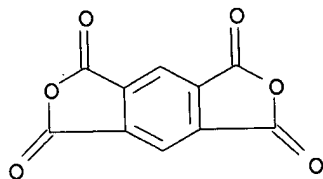
CMF C12 H4 D8 N2 O2 S



CM 2

CRN 89-32-7

CMF C10 H2 O6



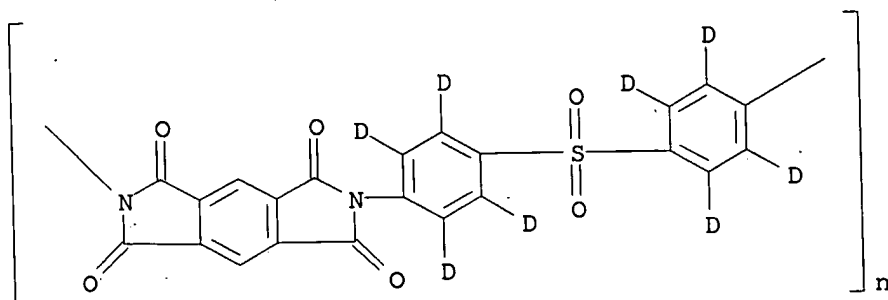
IT 870284-76-7P 870284-83-6P 870284-84-7P  
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870284-88-1P 870284-91-6P 870284-96-1P  
870284-97-2P 870286-98-9P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(high refractive index deuterated polyimides and derivs. with good transparency, low moisture absorption and optical transmission losses, heat resistance, and adhesion)

RN 870284-76-7 CAPLUS

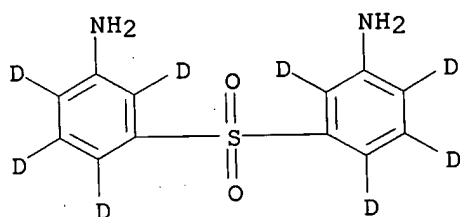
CN Poly[(5,7-dihydro-1,3,5,7-tetraoxobenzo[1,2-c:4,5-c']dipyrrole-2,6(1H,3H)-diyl)-1,4-phenylene-2,3,5,6-d4-sulfonyl-1,4-phenylene-2,3,5,6-d4] (9CI) (CA INDEX NAME)



RN 870284-83-6 CAPLUS  
 CN 1,3-Isobenzofurandione, 5,5'-carbonylbis-, polymer with  
 5,5'-sulfonylbis[benzen-2,3,4,6-d4-amine] (9CI) (CA INDEX NAME)

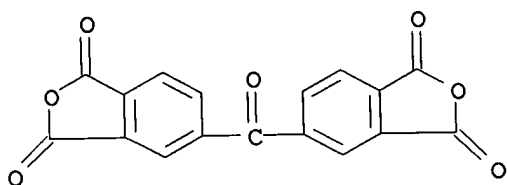
CM 1

CRN 870284-82-5  
 CMF C12 H4 D8 N2 O2 S

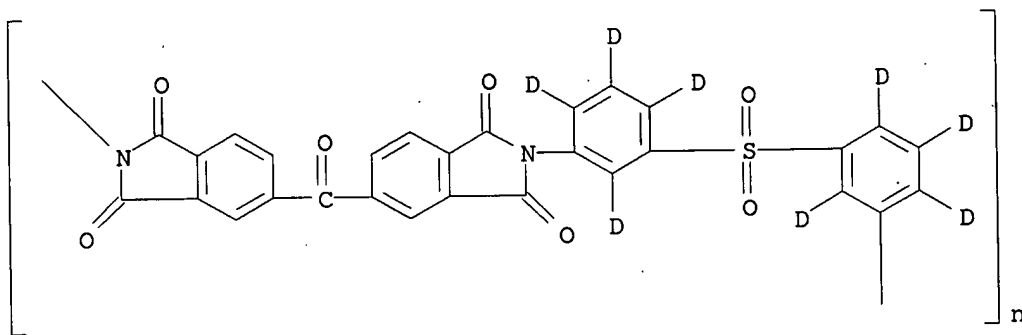


CM 2

CRN 2421-28-5  
 CMF C17 H6 O7

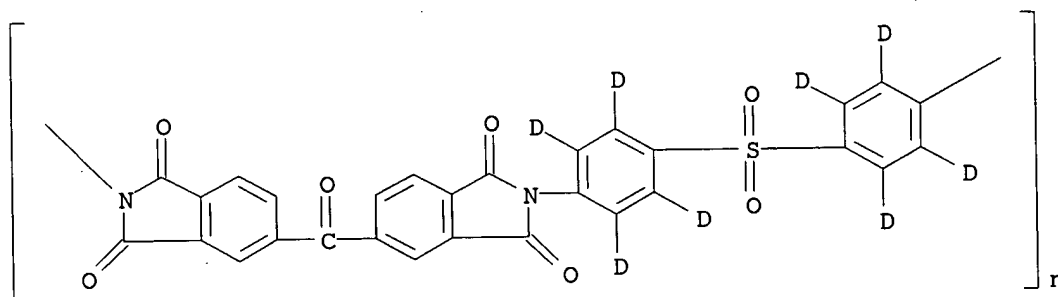


RN 870284-84-7 CAPLUS  
 CN Poly[(1,3-dihydro-1,3-dioxo-2H-isoindole-2,5-diyl)carbonyl(1,3-dihydro-1,3-dioxo-2H-isoindole-5,2-diyl)-1,3-phenylene-2,4,5,6-d4-sulfonyl-1,3-phenylene-2,4,5,6-d4] (9CI) (CA INDEX NAME)



RN 870284-85-8 CAPLUS

CN Poly[(1,3-dihydro-1,3-dioxo-2H-isoindole-2,5-diyl)carbonyl(1,3-dihydro-1,3-dioxo-2H-isoindole-5,2-diyl)-1,4-phenylene-2,3,5,6-d4-sulfonyl-1,4-phenylene-2,3,5,6-d4] (9CI) (CA INDEX NAME)



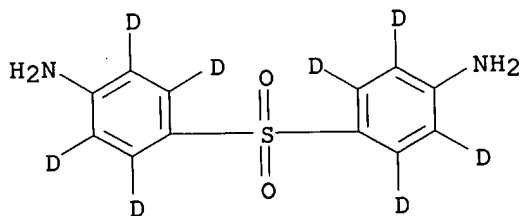
RN 870284-86-9 CAPLUS

CN 1,3-Isobenzofurandione, 5,5'-carbonylbis-, polymer with 4,4'-sulfonylbis[benzen-2,3,5,6-d4-amine] (9CI) (CA INDEX NAME)

CM 1

CRN 557794-38-4

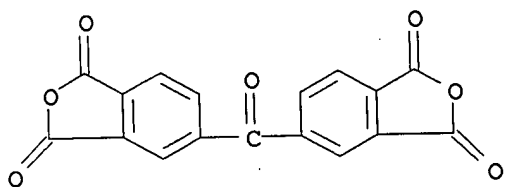
CMF C12 H4 D8 N2 O2 S



CM 2

CRN 2421-28-5

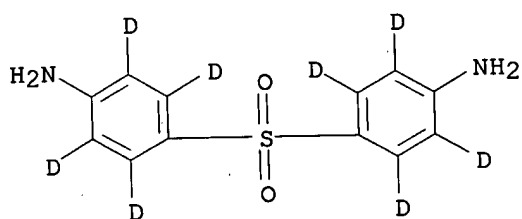
CMF C17 H6 O7



RN 870284-87-0 CAPLUS  
 CN [5,5'-Biisobenzofuran]-1,1',3,3'-tetrone, polymer with  
 4,4'-sulfonylbis[benzen-2,3,5,6-d4-amine] (9CI) (CA INDEX NAME)

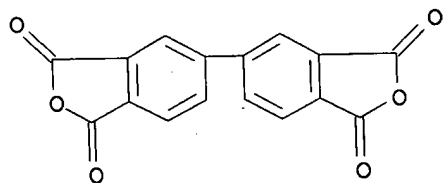
CM 1

CRN 557794-38-4  
 CMF C12 H4 D8 N2 O2 S



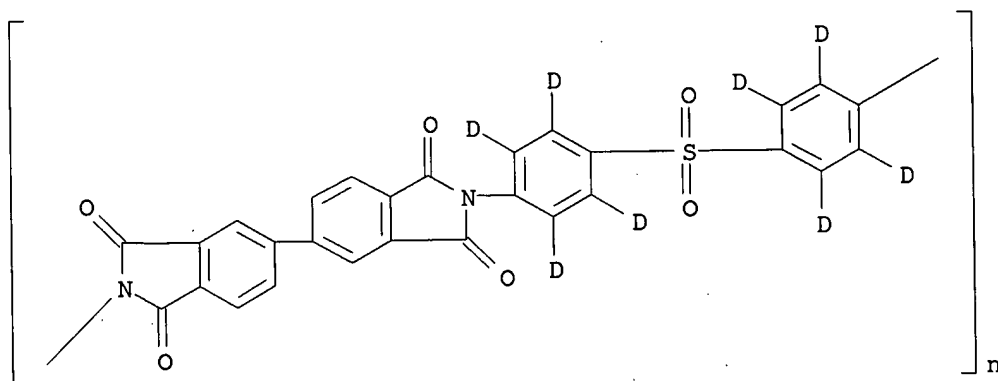
CM 2

CRN 2420-87-3  
 CMF C16 H6 O6



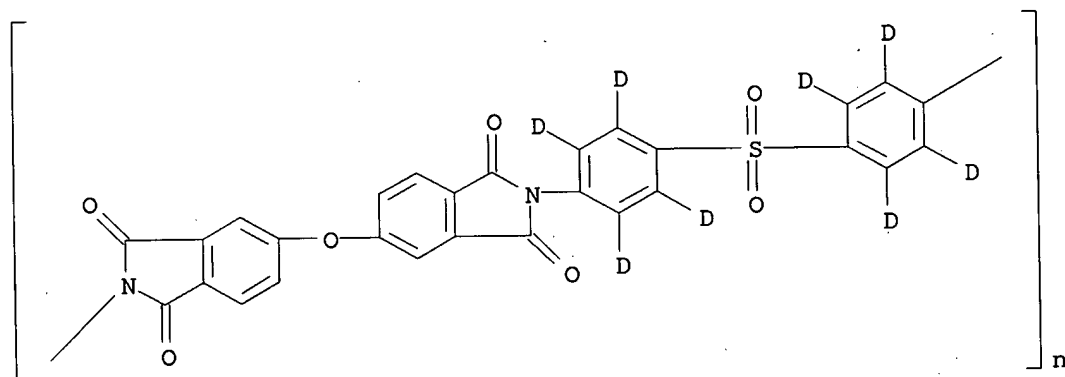
RN 870284-88-1 CAPLUS  
 CN Poly[(1,1',3,3'-tetrahydro-1,1',3,3'-tetraoxo[5,5'-bi-2H-isoindole]-2,2'-  
 diyl)-1,4-phenylene-2,3,5,6-d4-sulfonyl-1,4-phenylene-2,3,5,6-d4] (9CI)  
 (CA INDEX NAME)





RN 870284-91-6 CAPLUS

CN Poly[(1,3-dihydro-1,3-dioxo-2H-isoindole-2,5-diyl)oxy(1,3-dihydro-1,3-dioxo-2H-isoindole-5,2-diyl)-1,4-phenylene-2,3,5,6-d4-sulfonyl-1,4-phenylene-2,3,5,6-d4] (9CI) (CA INDEX NAME)



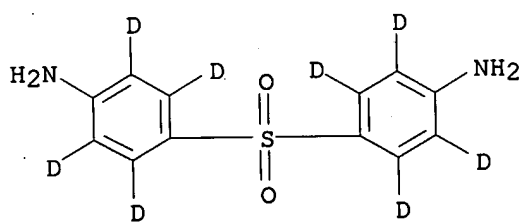
RN 870284-96-1 CAPLUS

CN Cyclobuta[1,2-c:3,4-c']difurantetrone, tetrahydro-, polymer with 4,4'-sulfonylbis[benzen-2,3,5,6-d4-amine] (9CI) (CA INDEX NAME)

CM 1

CRN 557794-38-4

CMF C12 H4 D8 N2 O2 S



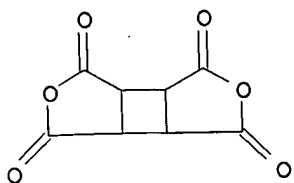
10/521,531

07/16/2008

CM 2

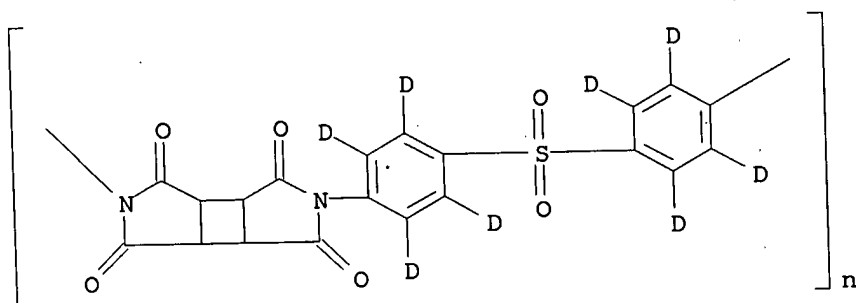
CRN 4415-87-6

CMF C8 H4 O6



RN 870284-97-2 CAPLUS

CN Poly[(octahydro-1,3,4,6-tetraoxocyclobuta[1,2-c:3,4-c']dipyrrole-2,5-diyl)-1,4-phenylene-2,3,5,6-d4-sulfonyl-1,4-phenylene-2,3,5,6-d4] (9CI) (CA INDEX NAME)



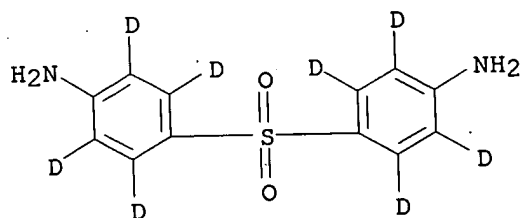
RN 870286-98-9 CAPLUS

CN 1,3-Isobenzofurandione, 5,5'-oxybis-, polymer with 4,4'-sulfonylbis[benzen-2,3,5,6-d4-amine] (9CI) (CA INDEX NAME)

CM 1

CRN 557794-38-4

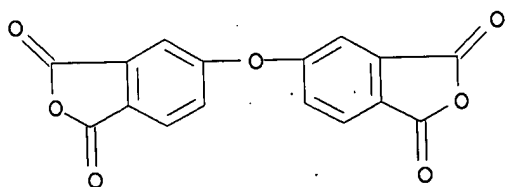
CMF C12 H4 D8 N2 O2 S



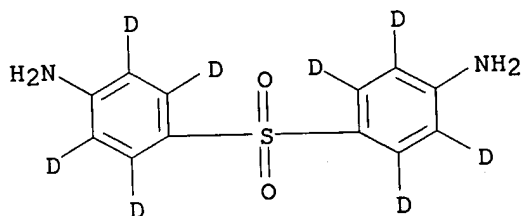
CM 2

CRN 1823-59-2

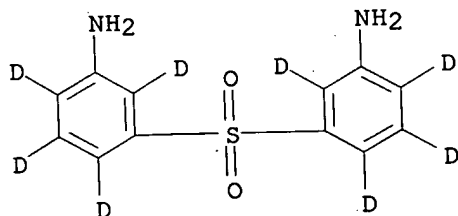
CMF C16 H6 O7



IT 557794-38-4P 870284-82-5P  
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (monomer; high refractive index deuterated polyimides and derivs. with  
 good transparency, low moisture absorption and optical transmission  
 losses, heat resistance, and adhesion)  
 RN 557794-38-4 CAPLUS  
 CN Benzen-2,3,5,6-d4-amine, 4,4'-sulfonylbis- (9CI) (CA INDEX NAME)



RN 870284-82-5 CAPLUS  
 CN Benzen-2,3,4,6-d4-amine, 5,5'-sulfonylbis- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

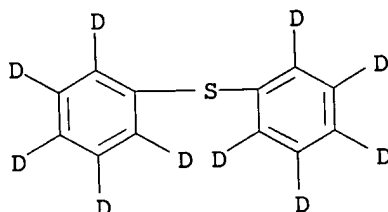
6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

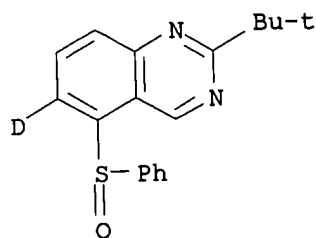
L3 ANSWER 6 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:1218389 CAPLUS  
 DOCUMENT NUMBER: 143:469300  
 TITLE: Multistep index plastic optical fiber  
 INVENTOR(S): Sasaki, Hiroki; Iwasaki, Osamu  
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005321686	A	20051117	JP 2004-140894	20040511
			JP 2004-140894	20040511

PRIORITY APPLN. INFO.:  
 AB The invention relates to a multistep index plastic optical fiber (POF) comprising coaxially placed  $\geq 3$  core layers made of an amorphous polymer composition that contains no C-H bonds and the cladding layer surrounding the core layers, wherein the distribution of the n's among the cores mimics that of GI-POF.  
 IT 180802-01-1  
 RL: DEV (Device component use); MOA (Modifier or additive use); USES (Uses)  
 (multistep index plastic optical fiber)  
 RN 180802-01-1 CAPLUS  
 CN Benzene-d<sub>5</sub>, 6,6'-thiobis- (9CI) (CA INDEX NAME)



L3 ANSWER 7 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:760273 CAPLUS  
 DOCUMENT NUMBER: 143:367265  
 TITLE: Metalation of sulfoxides in the benzodiazine series.  
 Diazines. Part 44  
 AUTHOR(S): Le Fur, Nicolas; Mojovic, Ljubica; Ple, Nelly; Turck, Alain; Marsais, Francis  
 CORPORATE SOURCE: Laboratoire de Chimie Organique Fine et Heterocyclique, IRCOF-INSA de Rouen, UMR CNRS 6014, Mont-Saint-Aignan, F-76131, Fr.  
 SOURCE: Tetrahedron (2005), 61(37), 8924-8931  
 CODEN: TETRAB; ISSN: 0040-4020  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 143:367265  
 AB The metalation of 12 benzodiazine sulfoxide derivs. was tested. This reaction was effective with 3-(sulfinyl)cinnoline derivs., 5-(phenylsulfinyl)-2-(tert-butyl)quinazoline and 8-[(tert-butyl)sulfinyl]-2-(tert-butyl)-4(3H)-quinazolinone. The reaction of 2-[(tert-butyl)sulfinyl]quinoxaline did not yield the desired products.  
 IT 866226-56-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (study of metalation of (tert-butyl)(phenylsulfinyl)quinazoline and subsequent electrophile trapping)  
 RN 866226-56-4 CAPLUS  
 CN Quinazoline-6-d, 2-(1,1-dimethylethyl)-5-(phenylsulfinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:487863 CAPLUS

DOCUMENT NUMBER: 143:34887

TITLE: Diphenylsulfide-containing polymers with low light transmission loss, good heat resistance, and high transmission band for optical components and plastic optical fibers

INVENTOR(S): Sasaki, Hiroki; Hatano, Seiji

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.

CODEN: JKXXAF

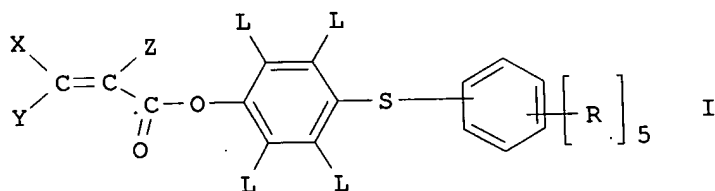
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005145861	A	20050609	JP 2003-383953	20031113
PRIORITY APPLN. INFO.:			JP 2003-383953	20031113
OTHER SOURCE(S):	MARPAT 143:34887			
GI				



AB Title polymers are obtained from diphenylsulfide compds. I, wherein X, Y = H, deuterium (D), or halogen; Z = H, D, Me, CD<sub>3</sub>, CF<sub>3</sub>, or halogen; and L, R = H, D, or substituent. Thus, 0.11 mol 4-mercaptophenol and 0.1 mol iodobenzene were reacted for 8 h, 0.05 mol of the resulting 4-phenylthiophenol was reacted with 0.055 mol acryloyl chloride to give 4-phenylthiophenoxy acrylate, which was mixed with Me methacrylate by varying composition, poured into a polymethyl methacrylate-coated KF 850 (polyvinylidene fluoride) tube with thickness 1 mm, inner diameter 22 mm, and length 30 cm, and polymerized at 80° while rotating the tube to give a hollow optical fiber preform with refractive index 1.420 in the cross

section direction (clad part), 1.490 (outer core part), and 1.490 - 1.501 (inner core part), which was stretched at 220-260° to give an optical fiber with light transmission loss 190 dB/km at 650 nm, transmission band 1.8 GHz, and glass transition temperature (core) 120°.

IT 852952-00-2P 852952-02-4P

RL: DEV (Device component use); IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(inner core layer; preparation of di-Ph sulfide-containing polymers with low light transmission loss, good heat resistance, and high transmission band for optical components and plastic optical fibers)

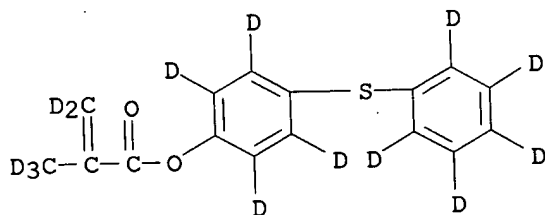
RN 852952-00-2 CAPLUS

CN 2-Propenoic-3,3-d2 acid, 2-(methyl-d3)-, methyl-d3 ester, polymer with 4-(phenyl-d5-thio)phenyl-2,3,5,6-d4 2-(methyl-d3)-2-propenoate-3,3-d2 (9CI) (CA INDEX NAME)

CM 1

CRN 852951-99-6

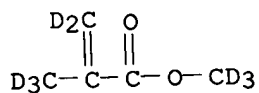
CMF C16 D14 O2 S



CM 2

CRN 35233-69-3

CMF C5 D8 O2



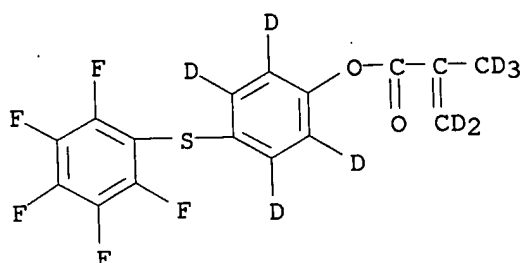
RN 852952-02-4 CAPLUS

CN 2-Propenoic-3,3-d2 acid, 2-(methyl-d3)-, 4-[(pentafluorophenyl)thio]phenyl-2,3,5,6-d4 ester, polymer with 2,2,2-trifluoroethyl-1,1-d2 2-(methyl-d3)-2-propenoate-3,3-d2 (9CI) (CA INDEX NAME)

CM 1

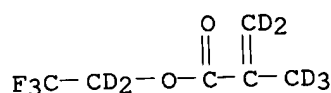
CRN 852952-01-3

CMF C16 D9 F5 O2 S



CM 2

CRN 697757-81-6  
CMF C6 D7 F3 O2



L3 ANSWER 9 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:405174 CAPLUS  
 DOCUMENT NUMBER: 141:54314  
 TITLE: Synthesis of 2-(arylthio)-3'-(alkyl- or dialkylamino)diphenyl sulfides via 5-arylthianthrenium perchlorates and their complexations with silver(I) and lead(II) ions  
 AUTHOR(S): Yoon, Kyongho; Kim, Kab Sig; Kim, Kyongtae  
 CORPORATE SOURCE: School of Chemistry and Molecular Engineering, Seoul National University, Seoul, 151-742, S. Korea  
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2003), (12), 138-163  
 CODEN: AGFUAR  
 URL: <http://www.arkat-usa.org/ark/journal/2003/Shine/H-S-868J/HS-868J.pdf>  
 PUBLISHER: Arkat USA Inc.  
 DOCUMENT TYPE: Journal; (online computer file)  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 141:54314  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Treatment of 5-arylthianthrenium perchlorates with secondary alkylamines in the presence of LDA in THF at reflux gave 2-(arylthio)-3'-(dialkylamino)diphenyl sulfides I as major products along with 2-(arylthio)-2'-(dialkylamino)diphenyl sulfides and thianthrene. The latter two compds. were formed depending on the structures of amines employed and the concns. of LDA. It has been found that the methoxy groups of I [X = MeO, Y = H; R = NPr<sub>2</sub> (II), morpholine, piperidine (III)]

were displaced by amide ions in the presence of excess amts. of LDA to give the corresponding 2-(4-dialkylaminophenylthio)-3'-(dialkylamino)diphenyl sulfides. The reactions with aza-15-crown-5, aza-18-crown-6, and 7, 16-diaza-18-crown-6 gave analogous products via a benzyne intermediate. The affinity of selected metal cations for compds. I [X = MeO, Y = H, R = NEt<sub>2</sub> (IV), NBu<sub>2</sub> (V), H (VI), N(iPr)<sub>2</sub> (VII)], II, III, VIII (X = MeO, iPrO), and IX was examined by an extraction method. The dialkylamino groups of II-V increased somewhat the extractive abilities of Ag<sup>+</sup> ion (14 - 28%) compared with that of VI (8%), whereas compound VII having a diisopropylamino group showed low (9%) and high (67%) extractive abilities toward Ag<sup>+</sup> and Pb<sup>2+</sup> ions, resp. Compds. VIII having an aza-18-crown-6 moiety showed 67% and 66% extractive abilities toward Pb<sup>2+</sup> but 40% and 24% extractive abilities towards Ag<sup>+</sup> ions, resp. However, compound IX with two identical lariats showed high (86%) and low (12%) extractive abilities toward Ag<sup>+</sup> and Pb<sup>2+</sup> ions, resp.

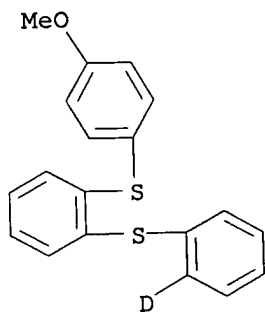
IT 709037-02-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (arylthio)-(alkyl- or dialkylamino)diphenyl sulfides via amination of arylthianthrenium perchlorates and evaluation of their extractive ability for metal cations)

RN 709037-02-5 CAPLUS

CN Benzene-d, 2-[[2-[(4-methoxyphenyl)thio]phenyl]thio]- (9CI) (CA INDEX NAME)



IT 709037-03-6P

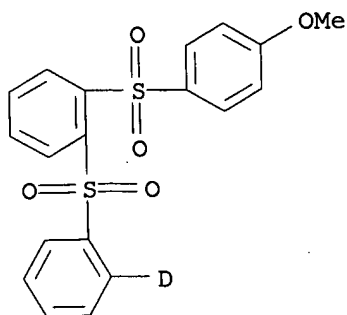
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of (arylthio)-(alkyl- or dialkylamino)diphenyl sulfides via amination of arylthianthrenium perchlorates and evaluation of their extractive ability for metal cations)

RN 709037-03-6 CAPLUS

CN Benzene-d, 2-[[2-[(4-methoxyphenyl)sulfonyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:346166 CAPLUS

DOCUMENT NUMBER: 141:47132

TITLE: Selectivity of 3H-MADAM binding to 5-hydroxytryptamine transporters in vitro and in vivo in mice; correlation with behavioral effects

AUTHOR(S): Larsen, A. K.; Brennum, L. T.; Egebjerg, J.; Sanchez, C.; Halldin, C.; Andersen, P. H.

CORPORATE SOURCE: Department of Disease Biology, H. Lundbeck A/S, Valby, DK-2500, Den.

SOURCE: British Journal of Pharmacology (2004), 141(6), 1015-1023

CODEN: BJPCBM; ISSN: 0007-1188

PUBLISHER: Nature Publishing Group

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Binding of the novel radioligand 3H-2-(2-dimethylaminomethyl-phenylsulfanyl)-5-methylphenylamine (3H-MADAM) to the serotonin transporter (SERT) was used to characterize a range of selective serotonin reuptake inhibitors (SSRIs) in vitro and in vivo. 3H-MADAM bound with high affinity in a saturable manner to both human SERT expressed in CHO cells ( $K_d=0.20$  nM ( $pK_d=9.74\pm0.12$ ),  $B_{max}=35\pm4$  fmol mg<sup>-1</sup> protein) and mouse cerebral cortex membranes ( $K_d=0.21$  nM ( $pK_d=9.66\pm0.10$ ),  $B_{max}=50\pm24$  fmol mg<sup>-1</sup> protein). Binding of 3H-MADAM was highly selective for SERT in vitro as demonstrated by the in vitro profile of MADAM tested at 75 different receptors, ion channels and transporters. This was further substantiated by the pharmacol. profile of the binding. Hence, the binding of 3H-MADAM was potently inhibited by SSRIs but not by selective inhibitors of noradrenaline transport and dopamine transport. Likewise, a 5-HT<sub>2A/2C</sub> receptor antagonist did not inhibit 3H-MADAM binding. 3H-MADAM binding in vivo was inhibited only by compds. which also inhibited the binding of 3H-MADAM in vitro (the SSRIs, mixed SERT/noradrenaline transport inhibitors and clomipramine), confirming the selectivity of 3H-MADAM for SERT also in vivo. Moreover, compds. effective in inhibiting 3H-MADAM binding were the only ones found to be active in the mouse 5-HTP potentiation test confirming the model as a behavioral correlate to in vivo 5-HT uptake. Finally, it was found that a SERT occupancy of 85-95% was necessary to produce 50% of the maximum behavioral response (ED<sub>50</sub>).

IT 708273-12-5

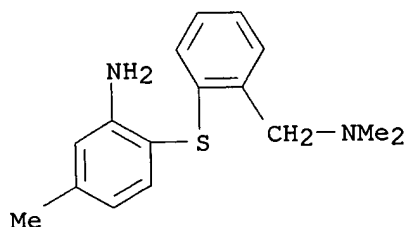
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological

study)

(selectivity of 3H-MADAM binding to 5-hydroxytryptamine transporters in vitro and in vivo in mice and correlation with behavioral effects)

RN 708273-12-5 CAPLUS

CN Benzenemethanamine, 2-[(2-amino-4-methylphenyl)thio]-N,N-dimethyl-, labeled with tritium (9CI) (CA INDEX NAME)



REFERENCE COUNT:

43

THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:190689 CAPLUS

DOCUMENT NUMBER: 139:100895

TITLE: Synthesis of deuterated 4,4'-diaminodiphenylsulfone (Dapsone) and related analogs

AUTHOR(S): Gannett, Peter M.; Johnson, Edward M., II; Grimes, Michael A.; Myers, Alan L.; Deavers, Robert E., III; Tracy, Timothy S.

CORPORATE SOURCE: Department of Basic Pharmaceutical Sciences, School of Pharmacy, West Virginia University, Morgantown, WV, 26506-9530, USA

SOURCE: Journal of Labelled Compounds &amp; Radiopharmaceuticals (2003), 46(2), 107-114

CODEN: JLCRD4; ISSN: 0362-4803

PUBLISHER: John Wiley &amp; Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:100895

AB A general scheme for the synthesis of 4,4'-diaminodiphenylsulfone-d<sub>5</sub> (Dapsone) from aniline-d<sub>5</sub> is described. The method may have general application and the preparation of the related analogs, 4,4'-dimethylaminodiphenyl sulfone from aniline-d<sub>5</sub> and 4,4'-dimethoxydiphenyl sulfone from phenol-d<sub>5</sub>, is also described.

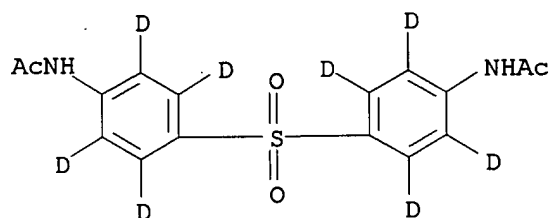
IT 557794-37-3P 557794-42-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(hydrolytic deprotection of; preparation of deuterated diaminodiphenylsulfone and related analogs using deuterated aniline and phenol as starting compds.)

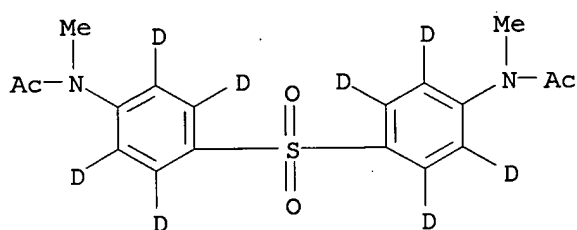
RN 557794-37-3 CAPLUS

CN Acetamide, N,N'-[sulfonyldi(4,1-phenylene-2,3,5,6-d<sub>4</sub>)]bis- (9CI) (CA INDEX NAME)



RN 557794-42-0 CAPLUS

CN Acetamide, N,N'-[sulfonyldi(4,1-phenylene-2,3,5,6-d4)]bis[N-methyl- (9CI)  
(CA INDEX NAME)]



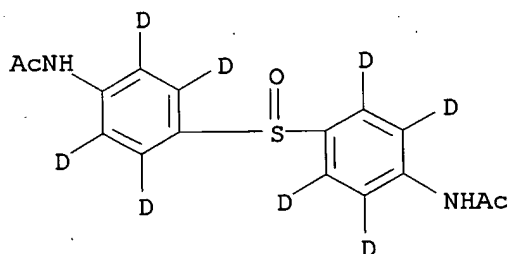
IT 557794-36-2P 557794-41-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(oxidation of; preparation of deuterated diaminodiphenylsulfone and related  
analogs using deuterated aniline and phenol as starting compds.)

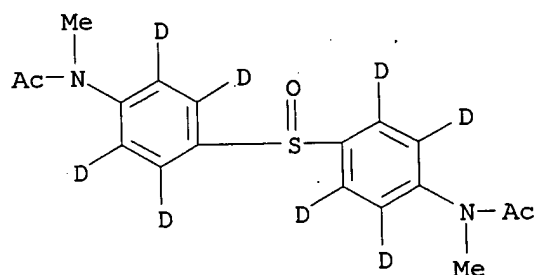
RN 557794-36-2 CAPLUS

CN Acetamide, N,N'-[sulfonyldi(4,1-phenylene-2,3,5,6-d4)]bis- (9CI) (CA  
INDEX NAME)



RN 557794-41-9 CAPLUS

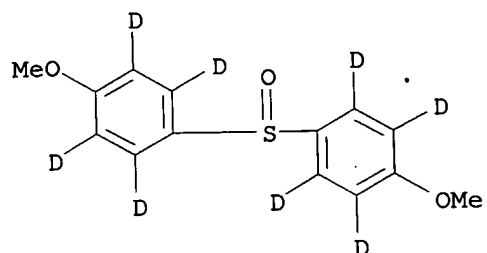
CN Acetamide, N,N'-[sulfonyldi(4,1-phenylene-2,3,5,6-d4)]bis[N-methyl- (9CI)  
(CA INDEX NAME)]



IT 557794-44-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (oxidation of; preparation of deuterated diaminodiphenylsulfone and related  
 analogs using deuterated aniline and phenol as starting compds.)

RN 557794-44-2 CAPLUS

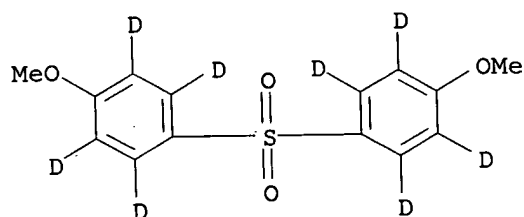
CN Benzene-1,2,4,5-d<sub>4</sub>, 3,3'-sulfinylbis[6-methoxy- (9CI) (CA INDEX NAME)

IT 557794-45-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation of deuterated diaminodiphenylsulfone and related analogs using  
 deuterated aniline and phenol as starting compds.)

RN 557794-45-3 CAPLUS

CN Benzene-1,2,4,5-d<sub>4</sub>, 3,3'-sulfonylbis[6-methoxy- (9CI) (CA INDEX NAME)

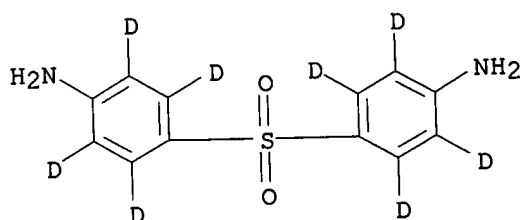
IT 557794-38-4P 557794-43-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

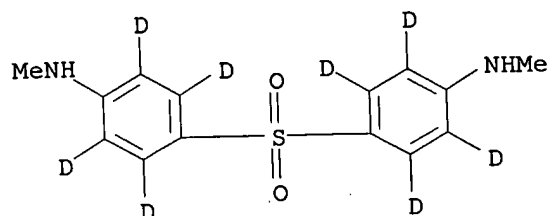
(preparation of deuterated diaminodiphenylsulfone and related analogs using  
 deuterated aniline and phenol as starting compds.)

RN 557794-38-4 CAPLUS

CN Benzen-2,3,5,6-d<sub>4</sub>-amine, 4,4'-sulfonylbis- (9CI) (CA INDEX NAME)



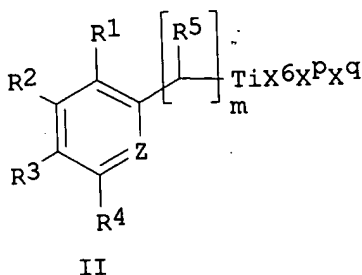
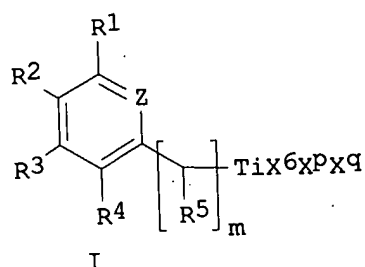
RN 557794-43-1 CAPLUS  
 CN Benzen-2,3,5,6-d4-amine, 4,4'-sulfonylbis[N-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:975678 CAPLUS  
 DOCUMENT NUMBER: 138:55870  
 TITLE: Regioselective preparation of organotitanium compounds and polysubstituted benzenes and pyridines  
 INVENTOR(S): Sato, Fumie  
 PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 33 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002371085	A	20021226	JP 2001-182554	20010615
US 20030096996	A1	20030522	US 2001-13453	20011213
US 6743916	B2	20040601		
US 20040167344	A1	20040826	US 2004-786150	20040226
US 7125999	B2	20061024		
PRIORITY APPLN. INFO.:			JP 2001-182554	A 20010615
			US 2001-13453	A3 20011213
OTHER SOURCE(S):			CASREACT 138:55870; MARPAT 138:55870	
GI				



AB The title compds. I [R1, R2 = C1-20 alkyl, C3-20 alkenyl, C1-6 alkoxy, C1-6 alkoxy carbonyl, etc.; R3, R4 = H, C1-20 alkyl, C1-6 alkoxy, C1-6 alkoxy carbonyl, C1-6 alkylaminocarbonyl, di(C1-6 alkyl)aminocarbonyl, etc.; R5 = H, C1-20 alkyl, (un)substituted phenyl; Z = CR', N; R' = H, C1-20 alkyl; X6 = halo, C1-6 alkoxy, phenoxy, naphthoxy, etc.; Xp, Xq = halo, (un)substituted C1-6 alkoxy, phenoxy, naphthoxy; m = 0-1] or II (R1-R5, Z, X6, m, Xp, Xq = same as I) are prepared by reaction of R1C.tplbond.CR2 (R1, R2 = same as I) with TiX1X2X3X4 [X1-X4 = halo, (un)substituted C1-6 alkoxy, phenoxy, naphthoxy], RMgX5 (R = C2-8 alkyl having H at  $\beta$ -position; X5 = halo), R3C.tplbond.CR4 (R3, R4 = same as I), and Z.tplbond.C(CHR5)mX6 (R5, m, X6 = same as I). Reaction of I and II, which were formed in situ, with electrophilic reagents such as aqueous HCl, O2, D2O, I2, CO2, PhCHO, etc., gives polysubstituted benzene and pyridine derivs. E.g., tert-Bu 2-nonynoate was reacted with isopropylmagnesium chloride and Ti(OPr-iso)4 in Et2O at -50° for 5 h and mixed with p-toluenesulfonylacetylene at room temperature for 3 h and quenched with aqueous HCl to give 50% [3-(tert-butoxycarbonyl)-4-hexylphenyl] p-tolyl sulfone.

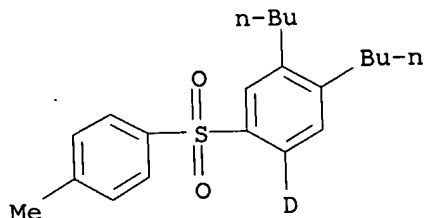
IT 360774-74-9P 360774-75-0P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(regioselective preparation of polysubstituted benzenes and pyridines by cycloaddn. of acetylenes in using Ti compds. and Grignard reagents)

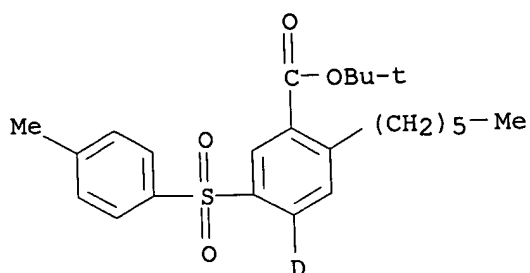
RN 360774-74-9 CAPLUS

CN Benzene-d, 4,5-dibutyl-2-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 360774-75-0 CAPLUS

CN Benzoic-4-d acid, 2-hexyl-5-[(4-methylphenyl)sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 13 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:970771 CAPLUS

DOCUMENT NUMBER: 139:62507

TITLE: Internal standard signal suppression by co-eluting analyte in isotope dilution LC-ESI-MS

AUTHOR(S): Sojo, Luis E.; Lum, Gina; Chee, Priscilla

CORPORATE SOURCE: Axelson BioPharma Research Inc., Burnaby, BC, V5G 1K5, Can.

SOURCE: Analyst (Cambridge, United Kingdom) (2003), 128(1), 51-54

CODEN: ANALAO; ISSN: 0003-2654

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The suppression of the internal standard by increasing concns. of the co-eluting analyte in calibration series and plasma samples analyzed by LC-ESI-MS was studied using the isotope dilution technique. A series of three analyte/deuterated analyte pairs including fexofenadine/d6-fexofenadine, dapsone/d4-dapsone and pseudoephedrine/d3-ephedrine were investigated. Suppression of the internal standard signal was noticed in extracted plasma samples containing fexofenadine and d6-fexofenadine as internal

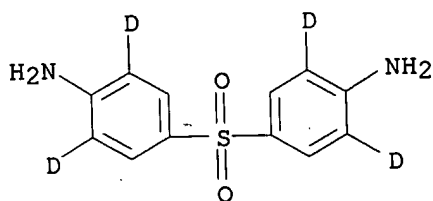
standard, as well as in solvent based calibration solns. of the three pair of compds. noted above during LC-ESI-MS anal. at flow rates greater than 100  $\mu\text{L min}^{-1}$ . This signal suppression effect was described by invoking Enke's model of electrospray ion generation. This model suggests that signal suppression can be ascribed to the competition between ionic species for charged surface sites present on the generated droplets during the electrospray process. The slopes of the calibration curves of the three analytes were close to unity (fexofenadine/d6-fexofenadine 0.964 $\pm$ 0.008, pseudoephedrine/d3-ephedrine 1.02 $\pm$ 0.080 and dapsone/d4-dapsone 0.905 $\pm$ 0.048) as predicted by the model, indicating that quantitation should not be affected by the variation in the peak area of the internal standard

IT 548783-72-8, d4-Dapsone

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (internal standard signal suppression by co-eluting analyte in human plasma samples analyzed by isotope dilution LC-ESI-MS)

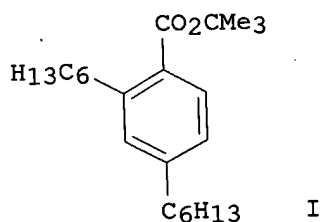
RN 548783-72-8 CAPLUS

CN Benzen-2,6-d2-amine, 4,4'-sulfonylbis- (9CI) (CA INDEX NAME)



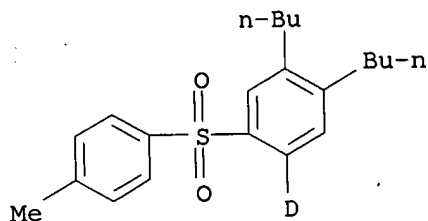
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:519718 CAPLUS  
 DOCUMENT NUMBER: 135:241952  
 TITLE: Metalative Reppe Reaction. Organized Assembly of Acetylene Molecules on Titanium Template Leading to a New Style of Acetylene Cyclotrimerization  
 AUTHOR(S): Suzuki, Daisuke; Urabe, Hirokazu; Sato, Fumie  
 CORPORATE SOURCE: Departments of Biomolecular Engineering and Biological Information Graduate School of Bioscience and Biotechnology, Tokyo Institute of Technology, Midori-ku Yokohama Kanagawa, 226-8501, Japan  
 SOURCE: Journal of the American Chemical Society (2001), 123(32), 7925-7926  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:241952  
 GI

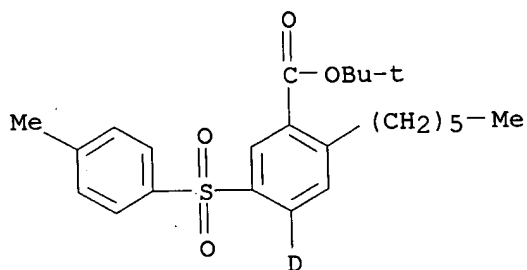


AB Three different, unsym. acetylenes and one mol. of ( $\eta^2$ -propene)Ti(O-i-Pr)<sub>2</sub> are combined together in a highly controlled manner to give acetylene trimers. E.g., reaction of Me<sub>3</sub>CO<sub>2</sub>CC.tplbond.CC<sub>6</sub>H<sub>13</sub>, 1-octyne, and ( $\eta^2$ -propene)Ti(O-i-Pr)<sub>2</sub>, followed by addition of ethynyl p-tolyl sulfone, gave benzene derivative I after hydrolysis.  
 IT 360774-74-9P 360774-75-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (metalative Reppe reaction of acetylene mols. on titanium template)  
 RN 360774-74-9 CAPLUS  
 CN Benzene-d, 4,5-dibutyl-2-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)





RN 360774-75-0 CAPLUS  
 CN Benzoic-4-d acid, 2-hexyl-5-[(4-methylphenyl)sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:395827 CAPLUS

DOCUMENT NUMBER: 135:129780

TITLE: 35Cl NQR and 2H NMR analysis of the critical dynamics by approaching from above the normal-incommensurate phase transition of bis(4-chlorophenyl)-sulfone (BCPS)

AUTHOR(S): Odin, C.; Meinel, C.; Etrillard, J.; Ollivier, J.; Toudic, B.

CORPORATE SOURCE: GMCM, Univ. Rennes I, Rennes, F-35042, Fr.

SOURCE: Ferroelectrics (2001), 250(1-4), 75-78

CODEN: FEROA8; ISSN: 0015-0193

PUBLISHER: Gordon & Breach Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

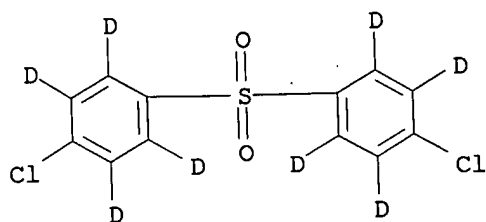
AB The inverse of the NQR or NMR spin lattice relaxation time of BCPS exhibits a Landau like critical behavior on approaching the normal/incommensurate phase transition from above. This critical behavior is interpreted as the contribution from the central peak observed in neutron expts. within the framework of the model of a coupling of the soft mode to pure relaxation modes. This result would be consistent with a central peak of dynamical nature.

IT 102438-60-8

RL: PEP (Physical, engineering or chemical process); PROC (Process) (spin-lattice relaxation study of normal-incommensurate phase transition of)

RN 102438-60-8 CAPLUS

CN Benzene-1,2,4,5-d4, 3,3'-sulfonylbis[6-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:323540 CAPLUS

DOCUMENT NUMBER: 133:83338

TITLE: Uranium(VI) Sulfilimine Complexes: A New Class of Nitrogen Analogues of the Uranyl Ion

AUTHOR(S): Williams, V. Cliff; Mueller, Matthias; Leech, Michael A.; Denning, Robert G.; Green, Malcolm L. H.

CORPORATE SOURCE: Inorganic Chemistry Laboratory, University of Oxford, Oxford, OX1 3QR, UK

SOURCE: Inorganic Chemistry (2000), 39(12), 2538-2541  
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB [Ph<sub>4</sub>P][UOCl<sub>4</sub>(NSPh<sub>2</sub>)] was prepared in high yield from [Ph<sub>4</sub>P][UOCl<sub>5</sub>] and Ph<sub>2</sub>S:NSiMe<sub>3</sub>. An x-ray structure of this compound shows that the U atom has a pseudooctahedral geometry with O and N atoms in trans positions. The structure of the analogous phosphoriminato complex [Ph<sub>4</sub>P][UOCl<sub>4</sub>(NPPh<sub>3</sub>)] was determined for comparison. Derivatization of the sulfide group shows that only a limited range of functionalization confers stability toward reduction. The emission spectrum of the 1st electronic excited state reveals a greatly reduced energy compared with that of the uranyl ion. This red shift in the transition is consistent with the weakening of the U-N bond relative to the U-O bond.

IT 278606-24-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and NMR)

RN 278606-24-9 CAPLUS

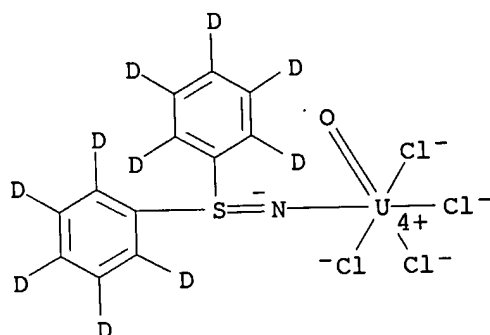
CN Phosphonium, tetraphenyl-, (OC-6-1,1)-tetrachloro[S,S-di(phenyl-d<sub>5</sub>)sulfiliminato-κN]oxouranate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 278606-23-8

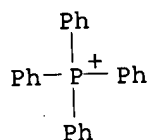
CMF C12 C14 D10 N O S U

CCI CCS



CM 2

CRN 18198-39-5  
CMF C24 H20 P



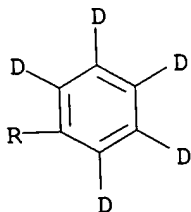
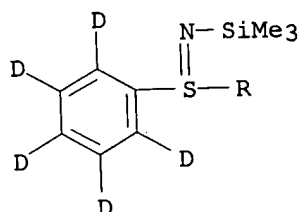
IT 278606-26-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for preparation of uranate sulfilimine oxo complexes)

RN 278606-26-1 CAPLUS

CN Sulfilimine, S,S-di(phenyl-d5)-N-(trimethylsilyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

23

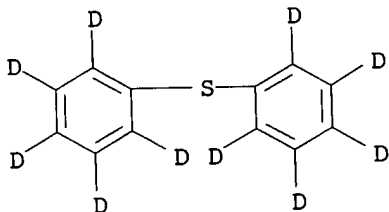
THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 17 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:143259 CAPLUS  
DOCUMENT NUMBER: 130:272291  
TITLE: Highly Mobile Solvent Holes in Viscous Squalane  
Solutions As Detected by Quantum Beats and MARY  
Spectroscopy Techniques. [Erratum to document cited in  
CA127:253377]  
AUTHOR(S): Usov, Oleg M.; Stass, Dmitrii V.; Tadjikov, Boris M.;  
Molin, Yuri N.  
CORPORATE SOURCE: Institute Chem. Kinetics and Combustion, Novosibirsk,  
630090, Russia  
SOURCE: Journal of Physical Chemistry A (1999), 103(11), 1690  
CODEN: JPFAFH; ISSN: 1089-5639  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB On page 7713, right column, line 15 from the top, "Expressions 3 and 4"  
should be replaced by "Expressions 4 and 5". On page 7714, left column,  
line 9 from the top, "expression 7" should read "expression 8".  
Correspondingly, in the same column, lines 15 and 16 from the bottom,  
instead of "eqs 3 and 4", it should be "eqs 4 and 5". In the right  
column, line 22 from the top, "expression 4" should be substituted by  
"expression 5". On page 7715, left column, line 1 from the top, "eq 3"  
should read "eq 4".

IT 180802-01-1, Diphenylsulfide-d10  
RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
PROC (Process)  
(highly mobile solvent holes in viscous squalane solns. as detected by  
quantum beats and MARY spectroscopy techniques (Erratum))  
RN 180802-01-1 CAPLUS  
CN Benzene-d5, 6,6'-thiobis- (9CI) (CA INDEX NAME)



L3 ANSWER 18 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:684171 CAPLUS  
DOCUMENT NUMBER: 129:347476  
ORIGINAL REFERENCE NO.: 129:70645a,70648a  
TITLE: Direct Observation of a Phason Gap in an  
Incommensurate Molecular Compound  
AUTHOR(S): Ollivier, J.; Etrillard, J.; Toudic, B.; Ecolivet, C.;  
Bourges, P.; Levanyuk, A. P.  
CORPORATE SOURCE: UMR au CNRS 6626, Groupe Matiere Condensee et  
Materiaux, Universite de Rennes 1, Campus de Beaulieu,  
Rennes, 35042, Fr.  
SOURCE: Physical Review Letters (1998), 81(17), 3667-3670  
CODEN: PRLTAO; ISSN: 0031-9007  
PUBLISHER: American Physical Society

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The results of an inelastic neutron scattering study of the lattice vibration spectra in the normal and incommensurate phases of  $(\text{ClC}_6\text{D}_4)_2\text{SO}_2$  are reported. Because of unusually low soft mode damping, a finite value of the phason frequency at the satellite position is observed for the first time. The soft mode frequency saturation in the normal phase and this phason gap are consistent with the dynamical nature of the observed central peak.

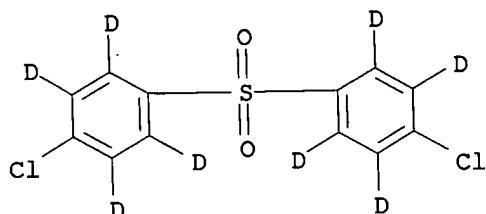
IT 102438-60-8

RL: PRP (Properties)

(direct observation of phason gap in incommensurate phase of)

RN 102438-60-8 CAPLUS

CN Benzene-1,2,4,5-d<sub>4</sub>, 3,3'-sulfonylbis[6-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:513415 CAPLUS

DOCUMENT NUMBER: 129:241003

ORIGINAL REFERENCE NO.: 129:48955a

TITLE: Disposition of diphenyl sulfoxide in rat

AUTHOR(S): Mitchell, S. C.; Gillham, J.; Jackson, W. F. M.;

Preston, S. L.; Porter, E. R.; Zhang, A. Q.

CORPORATE SOURCE: Molecular Toxicology, Division of Biomedical Sciences, Imperial College School of Medicine, London, W2 1PG, UK

SOURCE: Xenobiotica (1998), 28(7), 715-722

CODEN: XENOBH; ISSN: 0049-8254

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Radiolabeled di-Ph sulfoxide (U-14C- or 35S-) was administered by gavage (1.0 mmol/kg body weight) to the adult male Wistar rat following an overnight fast. For both labeled forms feces was the major route of excretion of radioactivity (50 %) with substantial amts. still being voided during the third and fourth days (13 %). Urinary elimination (42 %) was similar during the first (20 %) and second (17 %) days and a small amount of radioactivity (7 %) was found within the carcass after 4 days. Plasma data showed a peak concentration at 40 min (t<sub>max</sub>), a distribution half-life of

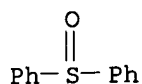
2

h (t<sub>1/2α</sub>) and an elimination half-life of 22.5 h (t<sub>1/2β</sub>).

Biliary studies revealed that 16 % of the dose traversed the bile duct during the first day with nearly half of this being excreted in the first 8 h. From urinary data, metabolism occurred via ring hydroxylation with subsequent conjugate formation. Oxidation of the sulfur to form the sulfone also took place. No evidence for sulfoxide reduction, cleavage of the ring

structures or exclusion of the sulfur was obtained.

IT 69490-45-5P  
 RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)  
 (disposition of di-Ph sulfoxide in rat)  
 RN 69490-45-5 CAPLUS  
 CN Benzene, 1,1'-sulfinylbis-, labeled with carbon-14 (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 20 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:61481 CAPLUS

DOCUMENT NUMBER: 128:167109

ORIGINAL REFERENCE NO.: 128:32932h,32933a

TITLE: Study of a fraction of spin-correlated pairs in radiation spurs by the methods of time-resolved magnetic field effects and quantum beats

AUTHOR(S): Anishchik, S. V.; Usov, O. M.; Anisimov, O. A.; Molin, Yu. N.

CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Novosibirsk, 630090, Russia

SOURCE: Radiation Physics and Chemistry (1997), Volume Date 1998, 51(1), 31-36

CODEN: RPCHDM; ISSN: 0969-806X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The fractions  $\Theta\beta$  and  $\Theta\chi$  of spin-correlated singlet radical-ion pairs in alkane solns. irradiated by  $\beta$ -particles and X-rays were got from expts. on magnetic field effect and quantum beats in recombination fluorescence. The ratio  $\Theta\beta/\Theta\chi$  values of 1.3-2.8 for the solvent series studied were found both from magnetic effect and quantum beats. The Monte Carlo calcns. were made to explain the variations of  $\Theta\beta/\Theta\chi$  in different solvents. The high value of  $\Theta\beta/\Theta\chi = 2.8$  for isooctane is probably due both to large separation between ions in pair and to high concentration of neutral radical in the spur.

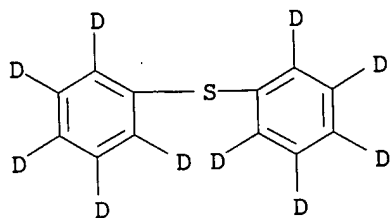
IT 180802-01-1

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(spin-correlated pairs in alkane solution irradiated by  $\beta$ -particles and x-rays)

RN 180802-01-1 CAPLUS

CN Benzene-d<sub>5</sub>, 6,6'-thiobis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:780055 CAPLUS

DOCUMENT NUMBER: 128:109790

ORIGINAL REFERENCE NO.: 128:21369a,21372a

TITLE: NMR structural analysis of incommensurate modulated systems with multiple active symmetry modes: A case study of deuterated bis(4-chlorophenyl)sulfone

AUTHOR(S): Meinel, C.; Zimmermann, H.; Haeberlen, U.; Etrillard, J.

CORPORATE SOURCE: AG Molekulkristalle, Max-Planck-Institut für Medizinische Forschung, Jahnstrasse 29, Heidelberg, 69120, Germany

SOURCE: Physical Review B: Condensed Matter (1997), 56(21), 13774-13784

CODEN: PRBMDO; ISSN: 0163-1829

PUBLISHER: American Physical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Single-crystal deutron NMR measurements both in the normal (N) and the incommensurate (IC) phase are reported for (4-ClC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>SO<sub>2</sub> (I). From the quadrupole-splitting data obtained in the N phase, the quadrupole coupling (QC) tensors of all deuterons in I are derived. The deutron NMR frequency distributions observed in the IC phase were analyzed as a function of the orientation of the applied magnetic field relative to the I crystal. This anal. is carried out in terms of the amplitudes and phases of the rotational-symmetry modes that contribute to the fundamental IC modulation wave in I, i.e., directly in terms of the structural changes associated with the IC phase transition. Both a semiquant. graphical, and a fully quant. numerical approach are given. The former is used to identify particularly simple and therefore particularly informative crystal orientations. The latter uses as an input the deutron QC tensors measured in the N phase. Quant. and complete structural information about the rotational displacements that atoms experience in an N-IC phase transition is deduced from NMR spectra. These results are in full agreement with the corresponding data from x-ray diffraction. Measurements of the spin-lattice relaxation time T<sub>1</sub> across the deutron NMR frequency distributions are also reported. The results are at variance with the established theory, and this is traced back to the fact that multiple rotational modes are contributing to the IC modulation wave in I.

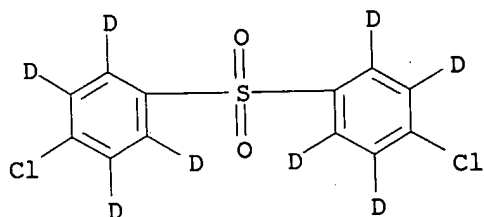
IT 102438-60-8 201361-64-0

RL: PRP (Properties)

(NMR structural anal. of incommensurate modulated systems with multiple active symmetry modes in deuterated bis(chlorophenyl)sulfone)

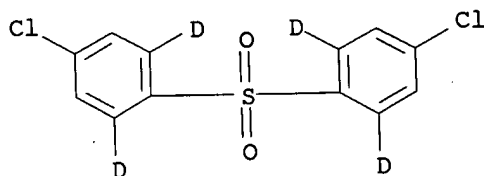
RN 102438-60-8 CAPLUS

CN Benzene-1,2,4,5-d4, 3,3'-sulfonylbis[6-chloro- (9CI) (CA INDEX NAME)



RN 201361-64-0 CAPLUS

CN Benzene-1,3-d2, 2,2'-sulfonylbis[5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

19

THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 22 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:623515 CAPLUS

DOCUMENT NUMBER: 127:253377

ORIGINAL REFERENCE NO.: 127:49413a,49416a

TITLE: Highly Mobile Solvent Holes in Viscous Squalane  
Solutions As Detected by Quantum Beats and MARY  
Spectroscopy TechniquesAUTHOR(S): Usov, Oleg M.; Stass, Dmitrii V.; Tadjikov, Boris M.;  
Molin, Yuri N.CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion,  
Novosibirsk, 630090, RussiaSOURCE: Journal of Physical Chemistry A (1997), 101(42),  
7711-7717

CODEN: JPFAFH; ISSN: 1089-5639

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The quantum beats and magnetic field effect on the reaction yield spectroscopy techniques were employed to study the formation of di-Ph sulfide radical cations in squalane solns. under ionizing irradiation It is demonstrated that the precursors of di-Ph sulfide radical cations are short-lived primary solvent radical cations (holes) with the ESR spectrum narrowed by the resonance charge transfer reaction. The rate constant of hole scavenging by di-Ph sulfide mols. was measured directly and amts. to  $6.1 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ , exceeding the diffusion-controlled one several times. The obtained value is well in line with the data on pulse radiolysis of squalane solns. with optical monitoring of the highly mobile precursor, supporting the hypothesis about the hole nature of the latter.

IT 180802-01-1, Diphenylsulfide-d10

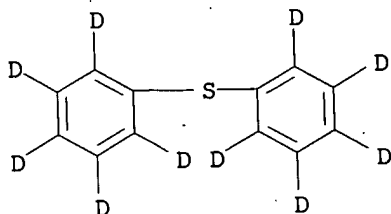


RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
PROC (Process)

(highly mobile solvent holes in viscous squalane solns. as detected by  
quantum beats and MARY spectroscopy techniques)

RN 180802-01-1 CAPLUS

CN Benzene-d<sub>5</sub>, 6,6'-thiobis- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

28

THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 23 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:575138 CAPLUS

DOCUMENT NUMBER: 127:242227

ORIGINAL REFERENCE NO.: 127:47099a,47102a

TITLE: Spin relaxation parameters in recombining radical ion

pair (diphenylsulfide-d<sub>10</sub>)/(p-terphenyl-d<sub>14</sub>)-  
obtained by ODESr and quantum beats techniques

AUTHOR(S):

Bagryansky, Victor A.; Usov, O. M.; Lukzen, N. N.;  
Molin, Y. N.

CORPORATE SOURCE:

Inst. Chemical Kinetics Combustion, Novosibirsk,  
630090, Russia

SOURCE:

Applied Magnetic Resonance (1997), 12(4), 505-512  
CODEN: APMREI; ISSN: 0937-9347

PUBLISHER:

Springer

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Parameters of paramagnetic relaxation were determined by OD (optically  
detected) ESR and quantum beats techniques for a recombining pair of  
radical ions (DPS-d<sub>10</sub>)/(PTP-d<sub>14</sub>)- (perdeuterated diphenylsulfide/p-  
terphenyl) in n-hexane, isooctane, cis-decalin, and squalane solns. The  
T<sub>2</sub> relaxation time determined by quantum beats technique is independent of  
solvent viscosity and magnetic field strength at 170-9600 G. These data  
agree with the results obtained by ODESr technique assuming fast T<sub>1</sub>  
relaxation for radical cation. Neglecting the contribution of radical  
anion relaxation T<sub>1c</sub> = T<sub>2c</sub> .simeq. 50 ns was obtained for (DPS-d<sub>10</sub>)+.

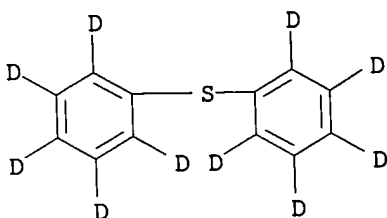
IT 180802-01-1

RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
PROC (Process)

(spin relaxation parameters in recombining radical ion pair  
(diphenylsulfide-d<sub>10</sub>)/(p-terphenyl-d<sub>14</sub>)- obtained by ODESr and quantum  
beats techniques)

RN 180802-01-1 CAPLUS

CN Benzene-d<sub>5</sub>, 6,6'-thiobis- (9CI) (CA INDEX NAME)



L3 ANSWER 24 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:120693 CAPLUS

DOCUMENT NUMBER: 126:199238

ORIGINAL REFERENCE NO.: 126:38515a,38518a

TITLE: Determination of a fraction of spin-correlated radical ion pairs in irradiated alkanes by quantum oscillation technique

AUTHOR(S): Usov, O. M.; Grigoryants, V. M.; Tadjikov, B. M.; Molin, Yu. N.

CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Novosibirsk, 630090, Russia

SOURCE: Radiation Physics and Chemistry (1997), 49(2), 237-243  
CODEN: RPCHDM; ISSN: 0146-5724

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Amplitudes of quantum oscillations observed in the recombination fluorescence of the (diphenylsulfide-d10)+/(p-terphenyl-d14)- radical ion pairs in alkane solns. have been used to estimate a fraction of spin-correlated singlet pairs  $\Theta$  in the radiation track.  $\Theta$  Values of 0.36 - 0.54 for the solvent series studied were found. Values for a fraction of singlet recombinations  $f_s$  (0.52-0.66), calculated from  $\Theta$  values, are in satisfactory agreement with those available from literature. It has been observed that  $\Theta$  and  $f_s$  values decrease with increasing solvent viscosity (from n-hexane to cis-decalin).

IT 180802-01-1, Diphenylsulfide-d10

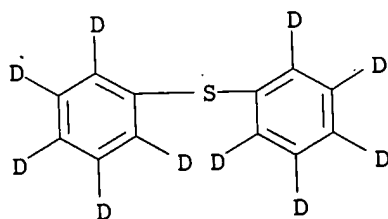
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(hole acceptor; determination of fraction of spin-correlated radical ion pairs

in irradiated alkanes by quantum oscillation technique)

RN 180802-01-1 CAPLUS

CN Benzene-d5, 6,6'-thiobis- (9CI) (CA INDEX NAME)



L3 ANSWER 25 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:74017 CAPLUS

DOCUMENT NUMBER: 126:205300

ORIGINAL REFERENCE NO.: 126:39579a,39582a

TITLE: Application of quantum oscillation technique for determination of the fraction of singlet

spin-correlated radical ion pairs during radiolysis

AUTHOR(S): Usov, O. M.; Grigor'yants, V. M.; Tadzhikov, B. M.; Molin, Yu. N.

CORPORATE SOURCE: Inst. Khim. Kinet. Gorennya, RAN, Novosibirsk, Russia

SOURCE: Doklady Akademii Nauk (1996), 349(6), 780-782

CODEN: DAKNEQ; ISSN: 0869-5652

PUBLISHER: MAIK Nauka

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Quantum oscillation technique was applied for determination of the fraction of singlet spin-correlated radical ion pairs and ratio of their singlet- and triplet recombination channels in ionizing radiation spurs.

IT 180802-01-1, Diphenylsulfide-d10

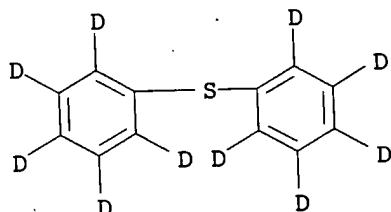
RL: PEP (Physical, engineering or chemical process); PROC (Process)

(application of quantum oscillation technique for determination of fraction

of singlet spin-correlated radical ion pairs produced in radiolysis)

RN 180802-01-1 CAPLUS

CN Benzene-d5, 6,6'-thiobis- (9CI) (CA INDEX NAME)



L3 ANSWER 26 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:369372 CAPLUS

DOCUMENT NUMBER: 125:180266

ORIGINAL REFERENCE NO.: 125:33533a,33536a

TITLE: Phase shift of quantum oscillations in the recombination luminescence of spin-correlated radical ion pairs

AUTHOR(S): Grigoryants, V. M.; Tadzhikov, B. M.; Usov, O. M.; Molin, Yu. N.

CORPORATE SOURCE: Institut Khimicheskoi Kinetiki i Gorennya, Novosibirsk, Russia

SOURCE: Doklady Akademii Nauk (1996), 346(4), 478-481

CODEN: DAKNEQ; ISSN: 0869-5652

PUBLISHER: MAIK Nauka

DOCUMENT TYPE: Journal

LANGUAGE: Russian

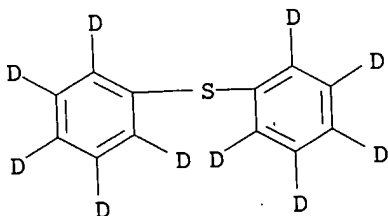
AB The phase shift of quantum oscillations of luminescence was observed in the recombination of singlet-correlated radical ion pairs of di-Ph sulfide and p-terphenyl ((DPS-d10)+/(PTP-d14)-). The shift is caused by the delay of (DPS-d10)+ appearance in the reaction of isooctane holes with (DPS-d10)

mol. As a result the rate constant of isooctane hole capture by (DPS-d10) mol. was obtained as  $(3.5 \pm 1) \cdot 10^{10} \text{ M}^{-1} \cdot \text{s}^{-1}$ .

IT 180802-01-1  
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
 (hole acceptor; phase shift of quantum oscillations in recombination luminescence of spin-correlated radical ion pairs)

RN 180802-01-1 CAPLUS

CN Benzene-d5, 6,6'-thiobis- (9CI) (CA INDEX NAME)



L3 ANSWER 27 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:961799 CAPLUS

DOCUMENT NUMBER: 124:17740

ORIGINAL REFERENCE NO.: 124:3283a, 3286a

TITLE: Phase shift of quantum oscillations in the recombination luminescence of spin-correlated radical ion pairs

AUTHOR(S): Grigoryants, V. M.; Tadjikov, B. M.; Usov, O. M.; Molin, Yu. N.

CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Novosibirsk, 630090, Russia

SOURCE: Chemical Physics Letters (1995), 246(4,5), 392-8  
 CODEN: CHPLBC; ISSN: 0009-2614

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

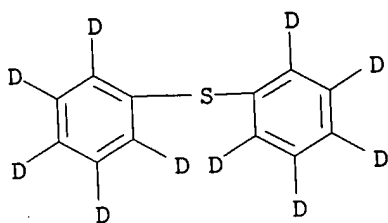
AB The phase shift of quantum oscillations observed in the recombination fluorescence of the (diphenylsulfide-d10)+/ (p-terphenyl-d14)- radical ion pair in isooctane has been detected exptl. The shift is caused by the delay in (diphenylsulfide-d10)+ formation in the reaction of solvent holes with a diphenylsulfide mol. Comparison with a theor. model has given for the rate constant of isooctane hole capture by diphenylsulfide mols. the value  $(3.5 \pm 1) \cdot 10^{10} \text{ M}^{-1} \text{ s}^{-1}$  which exceeds the diffusion-controlled one. The fraction of singlet-correlated pairs in the track has been estimated from the oscillation amplitude to be approx. 35%.

IT 171438-38-3

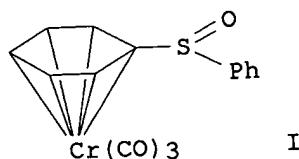
RL: PRP (Properties)  
 (phase shift of quantum oscillations in recombination luminescence of spin-correlated radical ion pairs)

RN 171438-38-3 CAPLUS

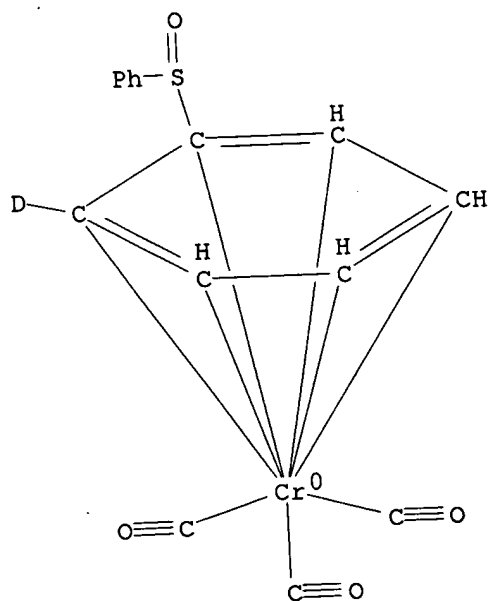
CN Benzene-d5, 6,6'-thiobis-, radical ion(1+) (9CI) (CA INDEX NAME)



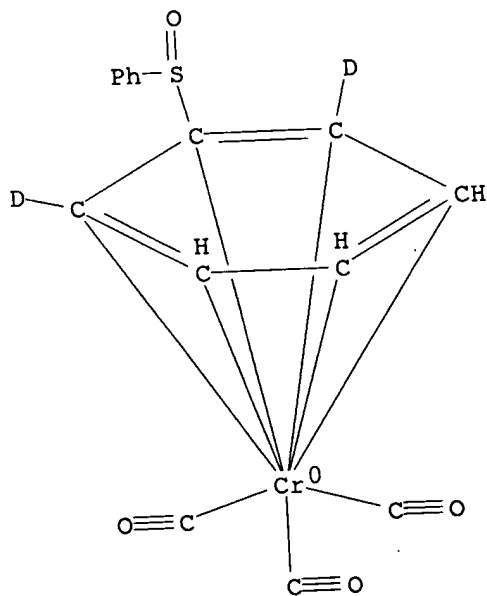
L3 ANSWER 28 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1995:542338 CAPLUS  
 DOCUMENT NUMBER: 123:144131  
 ORIGINAL REFERENCE NO.: 123:25685a,25688a  
 TITLE: Regioselective ortho substitution of diphenyl  
 sulfoxide chromium tricarbonyl: complementary  
 stereoselectivities for the mono- and di-anions  
 Davies, Stephen G.; Loveridge, Tracey; Clough, John M.  
 Dyson Perrins Laboratory, University Oxford, Oxford,  
 OX1 3QY, UK  
 AUTHOR(S):  
 CORPORATE SOURCE: Journal of the Chemical Society, Chemical  
 Communications (1995), (8), 817-18  
 SOURCE: CODEN: JCCCAT; ISSN: 0022-4936  
 Royal Society of Chemistry  
 PUBLISHER: Journal  
 DOCUMENT TYPE: English  
 LANGUAGE: CASREACT 123:144131  
 OTHER SOURCE(S):  
 GI



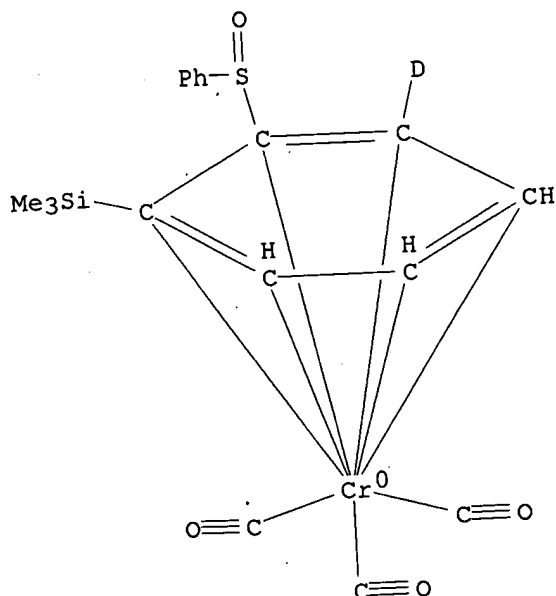
AB The mono- and di-anions derived from di-Ph sulfoxide Cr tricarbonyl I and  
 Li diisopropylamide show complementary stereoselectivities in their  
 reactions with electrophiles (D<sup>+</sup>, MeI, Me<sub>3</sub>SiCl).  
 IT 166192-33-2P 166192-35-4P 166192-38-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (complementary stereoselectivities for mono- and di-anions in  
 regioselective ortho substitution of di-Ph sulfoxide chromium  
 tricarbonyl)  
 RN 166192-33-2 CAPLUS  
 CN Chromium, tricarbonyl[(1,2,3,4,5,6-η)-2-(phenylsulfinyl)benzene-d]-,  
 stereoisomer (9CI) (CA INDEX NAME)



RN 166192-35-4 CAPLUS  
 CN Chromium, tricarbonyl[(1,2,3,4,5,6-η)-2-(phenylsulfinyl)benzene-1,3-d2]- (9CI) (CA INDEX NAME)



RN 166192-38-7 CAPLUS  
 CN Chromium, tricarbonyl[trimethyl[(1,2,3,4,5,6-η)-2-(phenylsulfinyl)phenyl-3-d]silane]-, stereoisomer (9CI) (CA INDEX NAME)



L3 ANSWER 29 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
 1994:667538 CAPLUS

ACCESSION NUMBER:

121:267538

DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.: 121:48629a, 48632a

TITLE:

Effect of Through-Space Interaction on the Photolytic  
 Desulfurization or Deselenization and Intramolecular  
 Cyclization Reactions of 1,9-Disubstituted  
 Dibenzochalcogenophenes

AUTHOR(S):

Kimura, Takeshi; Ishikawa, Yasuhiro; Ueki, Kensaku;  
 Horie, Yoji; Furukawa, Naomichi

CORPORATE SOURCE:

Department of Chemistry, University of Tsukuba,  
 Tsukuba, 305, Japan

SOURCE:

Journal of Organic Chemistry (1994), 59(23), 7117-24  
 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal  
 English

LANGUAGE:

OTHER SOURCE(S):

CASREACT 121:267538

AB

1,9-Dithia and 1,9-diselena substituents in dibenzochalcogenophenes (I) are in close proximity within the van der Waals S-S and Se-Se contacts and hence have a strong through-space interaction. Photolysis of the compds. (I) with a 400 W high-pressure mercury lamp in benzene produces triphenyleno[4,5-bcd]chalcogenophenes (II) and tribenzo[bc,e,hi][2,7]dichalcogenaazulenes (III) in high yields, except for the dibenzofuran derivative, via photoexcitation, sequential desulfurization or deselenization, and intramol. cyclization. In the reaction, 1,9-bis(phenylthio)dibenzofuran (Ie) exhibits lower reactivity as compared with other dibenzothiophene and dibenzoselenophene derivs. The X-ray crystallog. anal. of 1,9-bis(phenylseleno)dibenzoselenophene (Ia), 1,9-bis(phenylseleno)dibenzothiophene (Ib), and 1,9-bis(phenylthio)dibenzoselenophene (Ic) demonstrated that their structures are distorted as is also that of 1,9-bis(phenylthio)dibenzothiophene (Id), while dibenzofuran derivative Ie was found to be a nearly planar mol. The structure and reactivity relationship of compds. Ia-e was examined in the

photolytic reactions by comparing their interheteroat. distances at the 1,9 positions and their oxidation potentials. Furthermore, compds. Ia-e afforded the corresponding monosulfoxides and bis-sulfoxides on oxidation with m-chloroperbenzoic acid which were photolyzed readily to give also II and III.

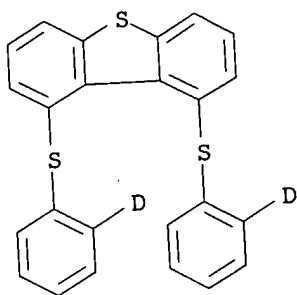
IT 149416-95-5 149416-96-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(photochem. desulfurization, deselenization and intramol. cyclization reactions of 1,9-disubstituted dibenzochalcogenophenes)

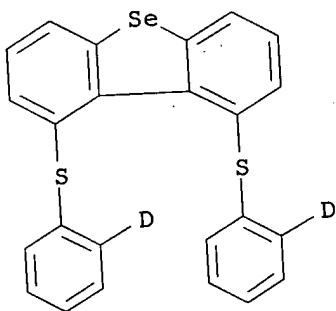
RN 149416-95-5 CAPLUS

CN Dibenzothiophene, 1,9-bis(phenyl-2-d-thio)- (9CI) (CA INDEX NAME)



RN 149416-96-6 CAPLUS

CN Dibenzoselenophene, 1,9-bis(phenyl-2-d-thio)- (9CI) (CA INDEX NAME)



L3 ANSWER 30 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:457251 CAPLUS

DOCUMENT NUMBER: 121:57251

ORIGINAL REFERENCE NO.: 121:10320h,10321a

TITLE: Simple preparation of sterically congested 1,9-disubstituted dibenzothiophenes and formation of their dithia dications via transannular S-S interaction

AUTHOR(S): Kimura, Takeshi; Horie, Yoji; Ogawa, Satoshi; Furukawa, Naomichi

CORPORATE SOURCE: Dep. Chem., Univ. Tsukuba, Tsukuba, 305, Japan

SOURCE: Heteroatom Chemistry (1993), 4(2-3), 243-52

DOCUMENT TYPE: CODEN: HETCE8; ISSN: 1042-7163

LANGUAGE: Journal

English

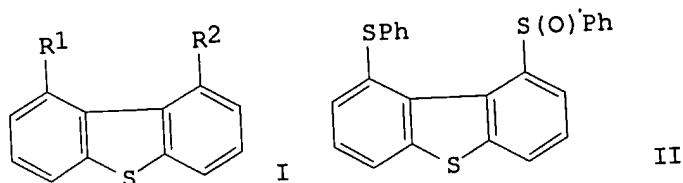


10/521,531

07/16/2008

OTHER SOURCE(S):  
GI

CASREACT 121:57251



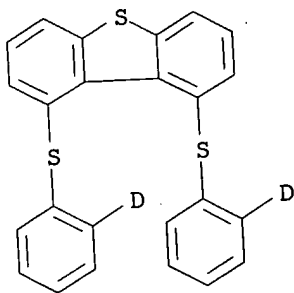
AB 4,6-Disubstituted thianthrene-5-oxides reacted with n-butyllithium to afford sterically crowded 1,9-disubstituted dibenzothiophenes (I; R1 = R2 = SPh, SC6H4Me-4, SMe, etc.; R2 = H, R1 = SPh, SC6H4Me-4) in moderate yields. The structures of the phenylthio derivative I (R1 = R2 = SPh) and its monooxide II were determined by x-ray crystallog. anal., which revealed that the distances between the two outer sulfur atoms are 3.012 Å (in I) and 3.016 Å (in II). I and their monoxides afforded the corresponding dithia dications on dissoln. in concentration sulfuric acid. The lower oxidation potentials of I compared with other dibenzothiophene derivs. reveal evidence for strong transannular interaction between the two outer sulfur atoms.

IT 149416-95-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 149416-95-5 CAPLUS

CN Dibenzothiophene, 1,9-bis(phenyl-2-d-thio)- (9CI) (CA INDEX NAME)



L3 ANSWER 31 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

1994:217054 CAPLUS

DOCUMENT NUMBER:

120:217054

ORIGINAL REFERENCE NO.:

120:38520h,38521a

TITLE:

Studies on dynemicin. A nonradical cycloaromatization pathway for the azabicyclo[7.3.1]enediynene core structure initiated by thiolate addition

AUTHOR(S):

Magnus, Philip; Eisenbeis, Shane A.; Rose, William C.; Zein, Nada; Solomon, Wyle

CORPORATE SOURCE:

Dep. Chem. Biochem., Univ. Texas, Austin, TX, 78712, USA

SOURCE:

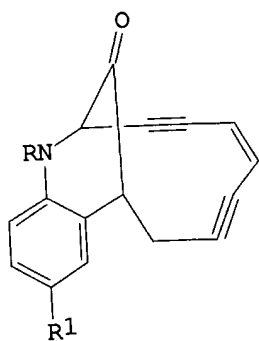
Journal of the American Chemical Society (1993), 115(26), 12627-8

07/16/200816/07/2008

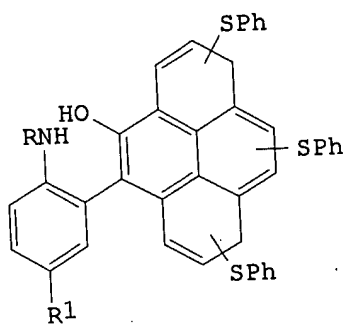
Page 49

DOCUMENT TYPE:  
LANGUAGE:  
GI

Journal  
English

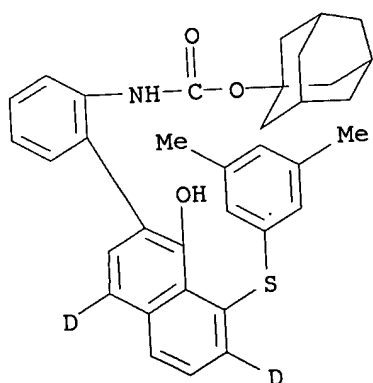


I



II

- AB The azabicyclododecenediyne I ( $R = R_1 = H$ ) and its derivs. I ( $R = CO_2CH_2CH_2Cl$ ,  $CO_2Me$ , adamantyloxycarbonyl,  $r_1 = H$ ) undergo Bergman cycloaromatization via a polar, non-radical pathway. I ( $R = R_1 = H$ ,  $OMe$ ) have antitumor activity in mice against P388 leukemia with T/C ratios of 175 and 170% resp. at 2mg/kg. I ( $R = R_1 = H$ ) was 350 times more potent than I ( $R =$  adamantyloxycarbonyl,  $R_1 = H$ ) against HCT116 human colon carcinoma, demonstrating that diradical formation is not required for antitumor activity.
- IT 154126-01-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)
- RN 154126-01-9 CAPLUS
- CN Carbamic acid, [2-[8-[(3,5-dimethylphenyl)thio]-1-hydroxy-2-naphthalenyl-4,7-d2]phenyl]-, tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl ester (9CI) (CA INDEX NAME)



L3 ANSWER 32 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1993:517398 CAPLUS  
DOCUMENT NUMBER: 119:117398  
ORIGINAL REFERENCE NO.: 119:21123a,21126a  
TITLE: Photochemical synthesis and electrochemical behavior

## AUTHOR(S):

CORPORATE SOURCE:  
SOURCE:

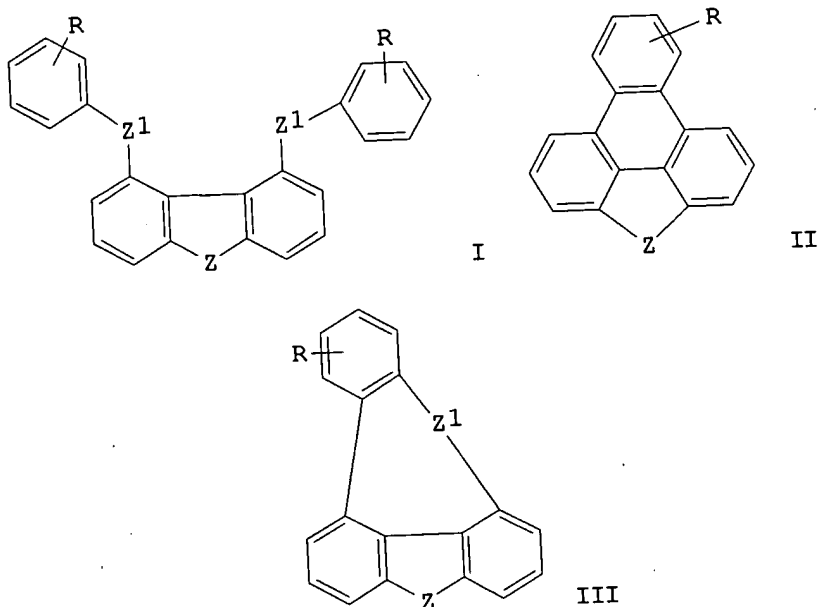
DOCUMENT TYPE:

LANGUAGE:

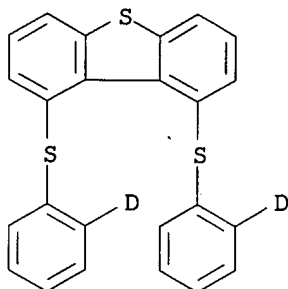
OTHER SOURCE(S):

GI

of triphenyleno[4,5-bcd]thiophene and  
triphenyleno[4,5-bcd]selenophene derivatives  
Kimura, Takeshi; Ishikawa, Yasuhiro; Furukawa,  
Naomichi  
Dep. Chem., Univ. Tsukuba, Tsukuba, 305, Japan  
Heterocycles (1993), 35(1), 53-6  
CODEN: HTCYAM; ISSN: 0385-5414  
Journal  
English  
CASREACT 119:117398

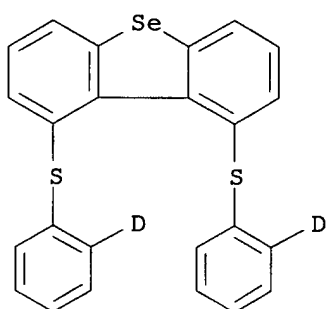


- AB Photolysis of 1,9-bis(arylthio)dibenzothiophenes (I, e.g., Z = Z1 = S, R = H, o-D, o-Me, p-Me, p-Cl) afforded corresponding triphenyleno[4,5-bcd]thiophenes II and tribenzo[bc,e,hi][2,7]dithiaazulenes III. A deuterium tracer experiment revealed that this reaction proceeded intramolecularly. Photolysis of 1,9-bis(arylseleno)dibenzoselenophene I (Z = Z1 = Se, R = H) afforded II (Z = Se, R = H) in 81% yield. The oxidation potentials of compds. II and III were measured by cyclic voltammetry.
- IT 149416-95-5 149416-96-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(intramol. photochem. cyclization of)
- RN 149416-95-5 CAPLUS
- CN Dibenzothiophene, 1,9-bis(phenyl-2-d-thio)- (9CI) (CA INDEX NAME)



RN 149416-96-6 CAPLUS

CN Dibenzoselenophene, 1,9-bis(phenyl-2-d-thio)- (9CI) (CA INDEX NAME)



L3 ANSWER 33 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:254809 CAPLUS

DOCUMENT NUMBER: 118:254809

ORIGINAL REFERENCE NO.: 118:44277a,44280a

TITLE: Synthesis of multiple carbon-14-labeled  
2,6-dichloro-3-nitrobenzoic acid and its incorporation  
in the synthesis of [14C]CI-958, a potential  
anticancer agent

AUTHOR(S): Huang, C. C.; Hicks, J. L.; Showalter, H. D. H.

CORPORATE SOURCE: Dep. Chem., Warner-Lambert Co., Ann Arbor, MI, USA

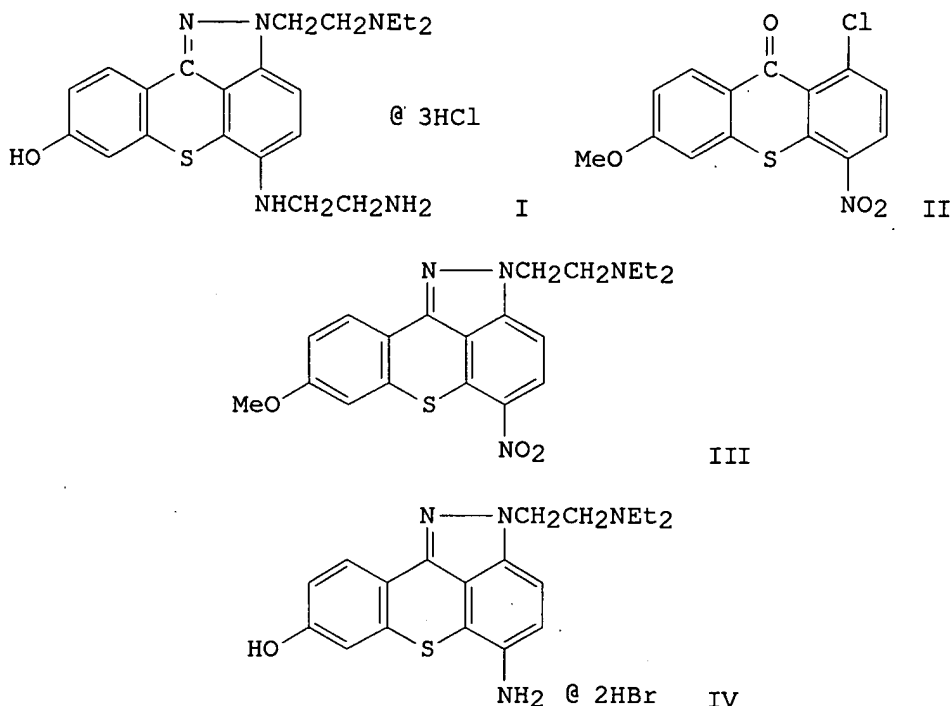
SOURCE: Synth. Appl. Isot. Labelled Compd. 1991, Proc. Int.  
Symp., 4th (1992), Meeting Date 1991, 187-92.Editor(s): Buncel, Erwin; Kabalka, George Walter.  
Elsevier: Amsterdam, Neth.

CODEN: 58MNAG

DOCUMENT TYPE: Conference

LANGUAGE: English

GI



AB CI-958 (I), a broad spectrum anticancer compound was multiple-labeled with carbon-14 using labeled 2,6-dichloro-3-nitrobenzoic acid as the key intermediate. [U-14C]benzene was dinitrated, reduced, diazotized, and subsequently chlorinated to give labeled 1,3-dichloro[U-14C]benzene. Metalation followed by carboxylation with  $^{14}\text{CO}_2$  produced the benzoic acid. Nitration yielded 2,6-dichloro-3-nitro[U-14C,carboxy-14C]benzoic acid. This was coupled with 3-methoxybenzenethiol and cyclized to give the [14C]-labeled 9H-thioxanthen-9-one II. Reaction with N,N-diethyl-2-hydrazinoethanamine gave the substituted 2H-[1]benzothiopyrano[4,3,2-cd]indazole III. The 5-nitro group was reduced, and the 8-methoxy was deprotected to give the 5-amino-N,N-diethyl-8-hydroxy-[10b-14C]2H-[1]benzothiopyrano[4,3,2-ce]-[U-14C]indazole-2-ethanamine dihydrobromide IV. The latter was coupled with N-triphenylmethylglycine activated with 1,1'-carbonyldiimidazole and the resulting amide was reduced, then deprotected to give [14C]-I.

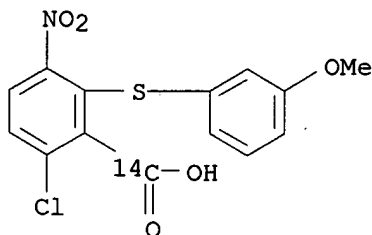
IT 147710-76-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and intramol. Friedel-Crafts acylation of, by thioxoanthenone from)

RN 147710-76-7 CAPLUS

CN Benzoic-carboxy-14C acid, 6-chloro-2-[(3-methoxyphenyl)thio]-3-nitro-, labeled with carbon-14 (9CI) (CA INDEX NAME)



L3 ANSWER 34 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:112391 CAPLUS

DOCUMENT NUMBER: 108:112391

ORIGINAL REFERENCE NO.: 108:18409a,18412a

TITLE: Fluorinated tricyclic neuroleptics with prolonged action: derivatives and analogs of 2-[4-(7-fluoro-2-isopropyl-10,11-dihydrodibenzo[b,f]thiepin-11-yl)piperazine-1-yl]ethanol

AUTHOR(S): Protiva, Miroslav; Jilek, Jiri; Rajsner, Miroslav; Sindelar, Karel; Bartl, Vaclav; Ryska, Miroslav; Koruna, Ivan; Holubek, Jiri; Svatek, Emil; et al.

CORPORATE SOURCE: Res. Inst. Pharm. Biochem., Prague, 130 60/3, Czech.  
SOURCE: Collection of Czechoslovak Chemical Communications (1987), 52(7), 1811-33

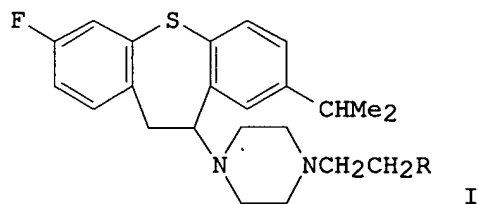
CODEN: CCCCAK; ISSN: 0366-547X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:112391

GI



AB Esterification of the neuroleptic agent, isofloxythepin, I (R = OH) (II) with Ac2O, decanoic acid, and 3,4,5-(MeO)3C6H2COCl gave esters, e.g., I (R = OAc) (III). Various analogs of II, e.g., I (R = CH2OH) (IV) and I (R = 1,3-dioxan-2-yl) (V) were also prepared. Pharmacol. testing of the analogs and derivs. of II for discoordinating and cataleptic activities showed very intensive and long-lasting effects for III, IV and V. I [R = O2C(CH2)8Me] has properties of a depot neuroleptic agent.

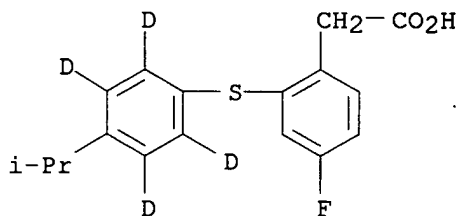
IT 113305-65-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of, dibenzothiepinone derivative from)

RN 113305-65-0 CAPLUS

CN Benzeneacetic acid, 4-fluoro-2-[[4-(1-methylethyl)phenyl-2,3,5,6-d4]thio]-(9CI) (CA INDEX NAME)



L3 ANSWER 35 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:55575 CAPLUS

DOCUMENT NUMBER: 108:55575

ORIGINAL REFERENCE NO.: 108:9269a,9272a

TITLE: Charge-transfer photooxygenation of sulfides in a cryogenic oxygen matrix. IR spectroscopic observation of persulfoxides

AUTHOR(S): Akasaka, Takeshi; Yabe, Akira; Ando, Wataru

CORPORATE SOURCE: Dep. Chem., Univ. Tsukuba, Sakura, 305, Japan

SOURCE: Journal of the American Chemical Society (1987), 109(26), 8085-7

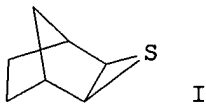
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:55575

GI



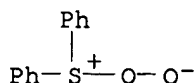
AB The photochem. reactions of MeSPh, Ph<sub>2</sub>S, and 3-thiatricyclo[3.2.1.0<sup>2,4</sup>]octane (I) in an oxygen matrix at 13 K were studied. The UV-visible absorption spectra reveal a contact charge-transfer (CT) band with a broad maximum at ca. 300 nm. The reaction intermediates resulting from UV irradiation (300-400 nm) of the contact CT band were studied by FT-IR spectroscopy. The first observation of the matrix-isolated persulfoxides, e.g., Ph<sub>2</sub>SO<sub>2</sub>, was achieved. Isotopic labeling expts. using <sup>18</sup>O<sub>2</sub> and <sup>16</sup>O<sub>2</sub> and 160-180 provided confirming evidence for the persulfoxide structure of the intermediates.

IT 111904-26-8P

RL: PRP (Properties); PREP (Preparation)  
(formation and IR spectrum of)

RN 111904-26-8 CAPLUS

CN Sulfonium, hydroperoxydiphenyl-, inner salt, labeled with oxygen-18 (9CI)  
(CA INDEX NAME)



L3 ANSWER 36 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:6760 CAPLUS

DOCUMENT NUMBER: 108:6760

ORIGINAL REFERENCE NO.: 108:1273a,1276a

TITLE: Synthesis and characterization of deuterated poly(arylene ether sulfones)

AUTHOR(S): Hedrick, J. L.; Dumais, J. J.; Jelinski, L. W.; Patsiga, R. A.; McGrath, J. E.

CORPORATE SOURCE: Almaden Res. Cent., IBM, San Jose, CA, 95120-6099, USA

SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry (1987), 25(8), 2289-300

CODEN: JPACEC; ISSN: 0887-624X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Selectively deuterated poly(arylene ether sulfones) were prepared for neutron scattering studies and for deuterium NMR investigations. The availability of these model macromols. permitted mol.-level identification of the motions responsible for the low-temperature relaxations that were observed

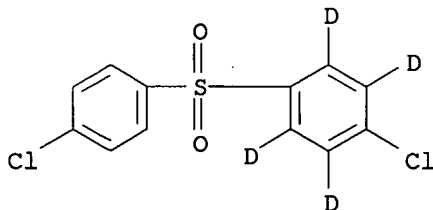
in the dynamic mech. spectra of these engineering polymers. Three labeled sites on the appropriate monomers (bisphenol A and 4,4'-dichlorodiphenyl sulfone) were prepared from deuterated intermediates and characterized via chromatog., spectroscopic, and thermal analyses. The deuterium exchange between Me and aromatic sites that occurred during synthesis was quantified. These labeled monomers were mixed with hydrogenous monomers to synthesize the high-mol.-weight title polymer. A synthetic technique involving N-methyl-2-pyrrolidone/K<sub>2</sub>CO<sub>3</sub> was employed to afford high-mol.-weight polymers. The polymers were characterized by Fourier-transform IR, proton, carbon, and deuterium NMR, intrinsic viscosities, and thermal anal. Mol. wts. of the labeled polymers were similar to unlabeled systems.

IT 92739-59-8P

RL: PREP (Preparation)  
(preparation and characterization of)

RN 92739-59-8 CAPLUS

CN Benzene-1,2,4,5-d<sub>4</sub>, 3-chloro-6-[(4-chlorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 37 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN



ACCESSION NUMBER: 1986:443645 CAPLUS  
DOCUMENT NUMBER: 105:43645  
ORIGINAL REFERENCE NO.: 105:7245a,7248a  
TITLE: Molecular basis of the  $\beta$ -transition in  
poly(arylene ether sulfones)  
AUTHOR(S): Dumais, J. J.; Cholli, A. L.; Jelinski, L. W.;  
Hedrick, J. L.; McGrath, J. E.  
CORPORATE SOURCE: AT and T Bell Lab., Murray Hill, NJ, 07974, USA  
SOURCE: Macromolecules (1986), 19(7), 1884-9  
CODEN: MAMOBX; ISSN: 0024-9297  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The mol. basis for the  $\beta$ -relaxation in poly(arylene ether sulfones) is established by deuterium NMR studies on specifically deuterated structures. The primary mode of motion of the aromatic rings in these polymers is  $180^\circ$  Ph ring flips. These flips occur with a broad distribution of characteristic frequencies (.apprx.102-107 s<sup>-1</sup>). Added antiplasticizers decrease the magnitude of the  $\beta$ -relaxation and lead to a significant loss in ductile mech. properties. Antiplasticizers also markedly reduce the rate of Ph ring flips, thereby establishing this type of Ph motion as a mol.-level process contributing to the  $\beta$ -relaxation. Other details of motion in these polymers are also addressed.

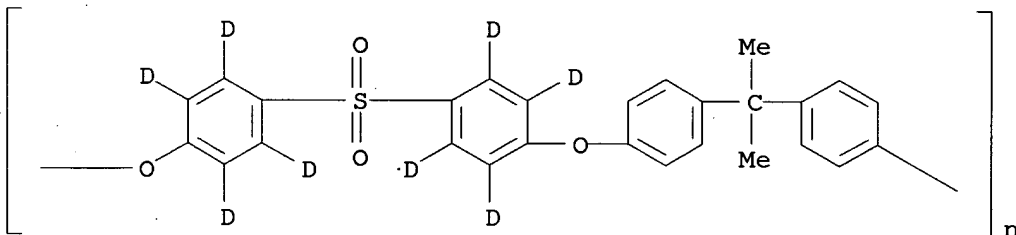
IT 102438-57-3 102438-61-9

RL: PROC (Process)

(relaxation of, mol. basis for)

RN 102438-57-3 CAPLUS

CN Poly[oxy-1,4-phenylene-2,3,5,6-d<sub>4</sub>-sulfonyl-1,4-phenylene-2,3,5,6-d<sub>4</sub>-oxy-1,4-phenylene(1-methylethylidene)-1,4-phenylene] (9CI) (CA INDEX NAME)



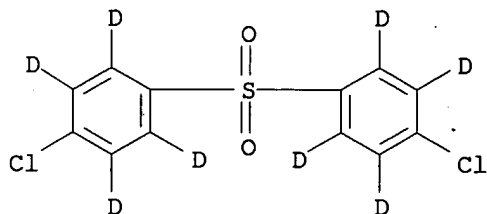
RN 102438-61-9 CAPLUS

CN Phenol, 4,4'-(1-methylethylidene)bis-, compd. with 3,3'-sulfonylbis[6-chlorobenzene-1,2,4,5-d<sub>4</sub>] (9CI) (CA INDEX NAME)

CM 1

CRN 102438-60-8

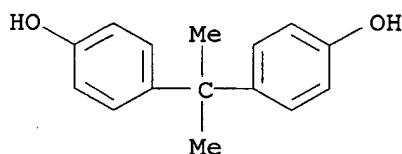
CMF C12 C12 D8 O2 S



CM 2

CRN 80-05-7

CMF C15 H16 O2



L3 ANSWER 38 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:181843 CAPLUS

DOCUMENT NUMBER: 102:181843

ORIGINAL REFERENCE NO.: 102:28479a,28482a

TITLE: Estimation of reserve albumin equivalent concentration for binding of bilirubin

AUTHOR(S): Brodersen, Rolf

CORPORATE SOURCE: Inst. Med. Biochem., Univ. Aarhus, Aarhus, DK-8000, Den.

SOURCE: Neonat. Jaundice, [Proc. Meet.] (1984), Meeting Date 1983, 55-61. Editor(s): Rubaltelli, Firmino F.; Jori, Giulio. Plenum: New York, N. Y.

CODEN: 53JUAL

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The determination of albumin bound to plasma bilirubin is discussed as a measure

of free bilirubin concentration and, thus, of plasma bilirubin toxicity, especially in

infants treated with sulfonamide for jaundice and respiratory distress.

The binding equilibrium of albumin, bilirubin, and their complexes with each other and sulfonamide were investigated. Albumin binding curves do not

have a level of saturation, but show a continuously upward trend. Thus, a new

parameter, the reserve albumin equivalent, is defined and the method was used

to measure reserve albumin concentration in infant plasma by using

[14C]monoacetyl diaminodiphenylsulfone in a dialysis experiment as a substitute for bilirubin.

IT 96156-35-3

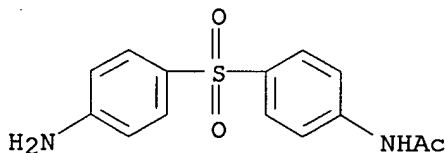
RL: ANST (Analytical study)

(in reserve albumin equivalent for bilirubin binding determination)

RN 96156-35-3 CAPLUS

CN Acetamide, N-[4-[(4-aminophenyl)sulfonyl]phenyl]-, labeled with carbon-14

(9CI) (CA INDEX NAME)



L3 ANSWER 39 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:571859 CAPLUS

DOCUMENT NUMBER: 101:171859

ORIGINAL REFERENCE NO.: 101:26009a,26012a

TITLE: Synthesis and characterization of deuterated poly(arylene ether sulfones)

AUTHOR(S): Hedrick, J. L.; Patsiga, R. A.; McGrath, J. E.

CORPORATE SOURCE: Dep. Chem. Polym. Mater., Virginia Polytech. Inst. and State Univ., Blacksburg, VA, 24061, USA

SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1984), 25(2), 88-90  
CODEN: ACPPAY; ISSN: 0032-3934

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Selectively deuterated bisphenol A (I) and 4,4'-dichlorodiphenyl sulfone were synthesized and used to prepare partially deuterated poly(arylene ether sulfone)s containing 3.5-20% D. M.ps. and Rf values from TLC anal. indicated that pure monomers (compared to com. samples) were prepared and structures were confirmed by NMR and Fourier-transform IR techniques. A D-exchange with the HCl catalyst produced partially deuterated I in which 50% of the isopropylidene linkages was deuterated or the Ph groups had D only in the 3,3',5, and 5' positions.

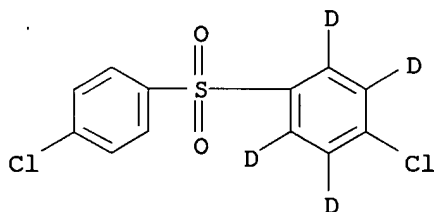
IT 92739-59-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and polymerization of, with bisphenol A and deuterated bisphenol A)

RN 92739-59-8 CAPLUS

CN Benzene-1,2,4,5-d4, 3-chloro-6-[(4-chlorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

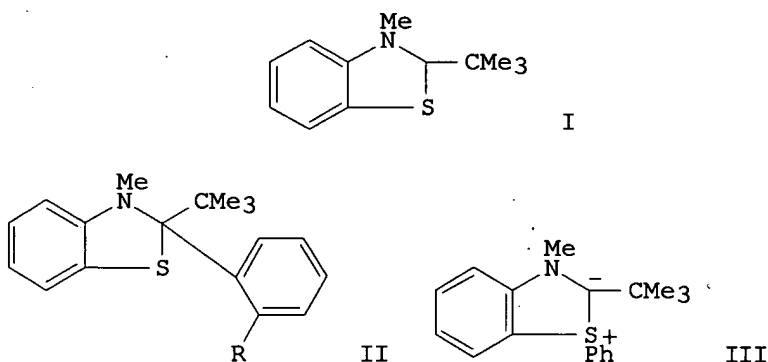


L3 ANSWER 40 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:52216 CAPLUS

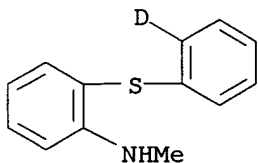
DOCUMENT NUMBER: 96:52216

ORIGINAL REFERENCE NO.: 96:8601a,8604a  
 TITLE: Reaction of benzothiazoline with benzyne. Generation of the novel heterocyclic sulfur ylide, benzothiazolinium S-ylide  
 AUTHOR(S): Hori, Mikio; Kataoka, Tadashi; Shimizu, Hiroshi; Ueda, Norihiro  
 CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, 502, Japan  
 SOURCE: Tetrahedron Letters (1981), 22(32), 3071-4  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 96:52216  
 GI

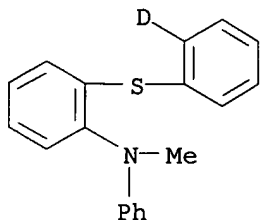


AB Reaction of the benzothiazoline I with benzyne, formed by treatment of o-BrC<sub>6</sub>H<sub>4</sub>F with Mg (room temperature, 4 h, THF), gave the benzothiazolines II (R = H, F) (34, 31%, resp.) and 18% o-PhSC<sub>6</sub>H<sub>4</sub>NHMe. The mechanism involved the formation of the heterocyclic S ylide III, which underwent a 1,2-intermol. shift to give II (R = H).

IT 80335-41-7P 80335-45-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 80335-41-7 CAPLUS  
 CN Benzenamine, N-methyl-2-(phenyl-2-d-thio)- (9CI) (CA INDEX NAME)



RN 80335-45-1 CAPLUS  
 CN Benzenamine, N-methyl-N-phenyl-2-(phenyl-2-d-thio)- (9CI) (CA INDEX NAME)



L3 ANSWER 41 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:121110 CAPLUS

DOCUMENT NUMBER: 90:121110

ORIGINAL REFERENCE NO.: 90:19163a,19166a

TITLE: Labeling of N-(2-diethylaminoethyl)-S,S-diphenylsulfoximine with carbon-14 in the side chain and the phenyl rings

AUTHOR(S): Liedtke, B.; Vollmer, K. O.

CORPORATE SOURCE: Abt. Biochem., Goedecke Res. Inst., Freiburg/Br., Fed. Rep. Ger.

SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1978), 14(6), 825-33

CODEN: JLCRD4; ISSN: 0362-4803

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 90:121110

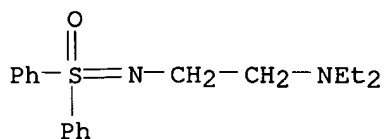
AB Ph2S(O):N14CH2CH2NEt2 was prepared (44.6% based on Ba14CO3) from acetic-carboxy-14C acid in 6 steps through substitution reaction of Et2NCH214CH2Cl with Ph2S(O):NH. Sequential treatment of C 14 labeled benzene with SOCl2-AlCl3, NaN3 in polyphosphoric acid, and Et2N(CH2)2Cl gave 30.4% Ph2S(O):N(CH2)2NEt2-phenyl-14C.

IT 69490-47-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 69490-47-7 CAPLUS

CN Sulfoximine, N-[2-(diethylamino)ethyl]-S,S-diphenyl-, labeled with carbon-14 (9CI) (CA INDEX NAME)

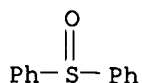


IT 69490-45-5P 69490-46-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as intermediate in carbon-14-labeled  
(diethylaminoethyl)diphenylsulfoximine preparation)

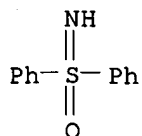
RN 69490-45-5 CAPLUS

CN Benzene, 1,1'-sulfinylbis-, labeled with carbon-14 (9CI) (CA INDEX NAME)



RN 69490-46-6 CAPLUS

CN Sulfoximine, S,S-diphenyl-, labeled with carbon-14 (9CI) (CA INDEX NAME)



L3 ANSWER 42 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:10233 CAPLUS

DOCUMENT NUMBER: 80:10233

ORIGINAL REFERENCE NO.: 80:1657a,1660a

TITLE: Metabolism of dapsone in man and experimental animals.  
Formation of N-hydroxy metabolitesAUTHOR(S): Israili, Z. H.; Cucinell, S. A.; Vaught, J.; Davis,  
E.; Lesser, J. M.; Dayton, P. G.

CORPORATE SOURCE: Sch. Med., Emory Univ., Atlanta, GA, USA

SOURCE: Journal of Pharmacology and Experimental Therapeutics  
(1973), 187(1), 138-51

CODEN: JPETAB; ISSN: 0022-3565

DOCUMENT TYPE: Journal

LANGUAGE: English

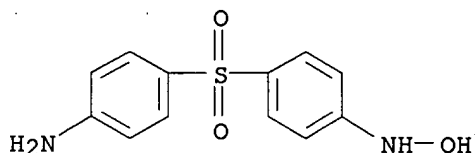
AB In human subjects receiving oral doses of labeled dapsone (I) [80-08-0] or diformyl dapsone (II) [6784-25-4], N-oxidation was a major metabolic route and the urine was a major excretory route. One of the primary urinary N-oxidation metabolites was characterized as azoxydapsone [35040-12-1]. A new metabolite, 4-acetylamino-4'-hydroxylaminodiphenylsulfone [32604-86-7], was also identified. The blood plasma half-life was about 1 day for both I and II. N-oxidation metabolites accounted for a small fraction of the I dose in the urine and liver of guinea pigs and rats; the amount in the bile was higher. Of the various I metabolites and derivs. tested, only the hydroxylamines were significantly active in producing methemoglobin in vitro. As would be expected from their lipid solubility, I and 4-amino-4'-hydroxyaminodiphenylsulfone [32695-27-5] rapidly penetrated into isolated human erythrocytes.

IT 50444-14-9P

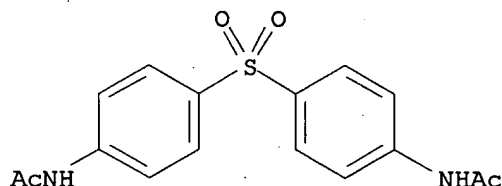
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 50444-14-9 CAPLUS

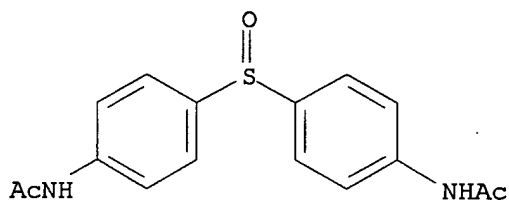
CN Benzenamine, 4-[(4-aminophenyl)sulfonyl]-N-hydroxy-, labeled with tritium  
(9CI) (CA INDEX NAME)



L3 ANSWER 43 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1972:405095 CAPLUS  
 DOCUMENT NUMBER: 77:5095  
 ORIGINAL REFERENCE NO.: 77:895a,898a  
 TITLE: Synthesis and characterization of carbon-14 labeled 4,4'-diaminodiphenyl sulfone (dapsone-14C; DDS-14C)  
 AUTHOR(S): Blackburn, C. E.; Glazko, A. J.  
 CORPORATE SOURCE: Dep. Pharmacol., Parke-Davis Co., Ann Arbor, MI, USA  
 SOURCE: Journal of Labelled Compounds (1972), 8(1), 63-70  
 CODEN: JLCAAI; ISSN: 0022-2135  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB ,4'-Diaminodiphenyl-14C sulfone was prepared in 4 steps from uniformly 14C-labeled aniline-HCl via acetanilide-phenyl-14C, 4,4'-bisacetamidodiphenyl-14C sulfoxide, and 4,4'-bisacetami-dodiphenyl-14C sulfone.  
 IT 36639-38-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrolysis of)  
 RN 36639-38-0 CAPLUS  
 CN Acetamide, N,N'-(sulfonyldi-4,1-phenylene)bis-, labeled with carbon-14 (9CI) (CA INDEX NAME)



IT 36639-37-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (oxidation of, sulfone from)  
 RN 36639-37-9 CAPLUS  
 CN Acetamide, N,N'-(sulfonyldi-4,1-phenylene)bis-, labeled with carbon-14 (9CI) (CA INDEX NAME)

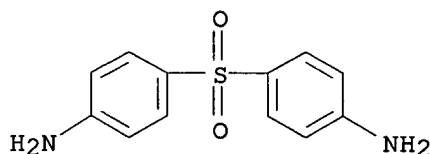


IT 36639-39-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 36639-39-1 CAPLUS

CN Benzenamine, 4,4'-sulfonylbis-, labeled with carbon-14 (9CI) (CA INDEX NAME)



L3 ANSWER 44 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:459482 CAPLUS

DOCUMENT NUMBER: 71:59482

ORIGINAL REFERENCE NO.: 71:10935a,10938a

TITLE: Whole-body autoradiographic studies on the distribution of radioisotopes. XVI. Distribution of tritium labeled new antitoxoplasmic agent, 2-sulfamoyl-4,1-diaminodiphenyl sulfone (3H-SDDS) in mice

AUTHOR(S): Sakuma, Mari; Sato, Yoshishige

CORPORATE SOURCE: Tanabe Seiyaku Co., Ltd., Japan

SOURCE: Radioisotopes (1969), 18(4), 143-7

CODEN: RAISAB; ISSN: 0033-8303

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB SDDS-3H (I) was administered i.p., orally, and i.m. into mice and its distribution in the body was examined by whole-body autoradiography. The rate of distribution of the radioactivity was greater by oral and i.p. administration than by i.m.; the activities were distributed evenly in all the organs and tissues, except in the central nervous system; maximum incorporation occurred in 3-5 hrs. after its administration, followed by loss of the activity in 24 hrs. It was excreted mainly through bile and urine. The activity of I was also distributed evenly in the tissues of the fetus and placenta.

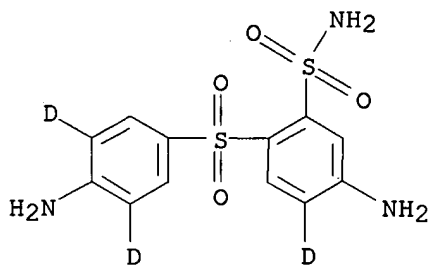
IT 25451-80-3

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(metabolism of)

RN 25451-80-3 CAPLUS

CN Metanilamide-4-d, 6-(sulfanilyl-3,5-d2)- (8CI) (CA INDEX NAME)





L3 ANSWER 45 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:511681 CAPLUS

DOCUMENT NUMBER: 69:111681

ORIGINAL REFERENCE NO.: 69:20919a,20922a

TITLE: Infrared spectra of benzene- and pentadeuterobenzenesulfonyl compounds

AUTHOR(S): Uno, Toyozo; Machida, Katsunosuke; Hanai, Kazuhiko

CORPORATE SOURCE: Fac. Pharm. Sci., Kyoto Univ., Kyoto, Japan

SOURCE: Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (1968), 24(11), 1705-12  
CODEN: SAMCAS; ISSN: 1386-1425

DOCUMENT TYPE: Journal

LANGUAGE: English

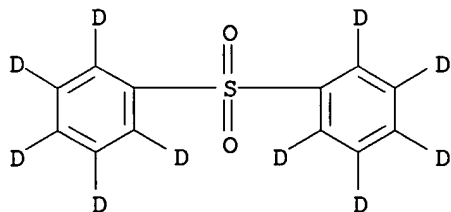
AB The ir spectra 4000-400 cm.<sup>-1</sup> of benzenesulfonamide, benzenesulfonanilide, benzenesulfonyl chloride, and diphenyl sulfone are reported together with the spectra of the corresponding pentadeuterobenzenesulfonyl compds. The isotopic shift of the characteristic bands near 1090 cm.<sup>-1</sup> of benzenesulfonyl compds. gives evidence of the assignment of this band to a mixed mode of the C-S stretching and a ring skeletal vibration. The benzene and deuterobenzene ring frequencies of these compds. are in close correspondence with those of chlorobenzene and chlorobenzene-d5. The effects of the N-deuteration and the ring deuteration on the SO<sub>2</sub> group frequencies are discussed.

IT 21885-27-8

RL: PRP (Properties)  
(spectrum (ir) of)

RN 21885-27-8 CAPLUS

CN (Phenyl sulfone)-d10 (8CI) (CA INDEX NAME)



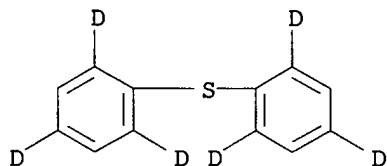
L3 ANSWER 46 OF 46 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1968:476394 CAPLUS

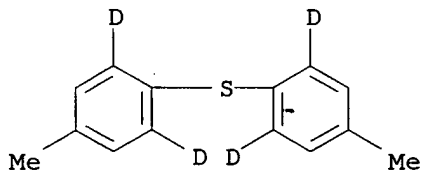
DOCUMENT NUMBER: 69:76394

ORIGINAL REFERENCE NO.: 69:14251a,14254a

TITLE: Skeletal rearrangements in mass spectra. I. Bis-aryl compounds  
AUTHOR(S): Wszolek, P. C.; McLafferty, F. W.; Brewster, J. H.  
CORPORATE SOURCE: Purdue Univ., Lafayette, IN, USA  
SOURCE: Organic Mass Spectrometry (1968), 1(1), 127-37  
CODEN: ORMSBG; ISSN: 0030-493X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Examination of a large number of spectra indicates that diunsatd. compds. commonly undergo a skeletal rearrangement in which part or all of the bridging moiety is eliminated, often with concomitant loss of H atoms. The spectra of labeled azobenzene, Ph<sub>2</sub>S, and their p,p'-dimethyl derivs. show that scrambling of H atoms precedes or accompanies such rearrangements, in contrast to the loss of a p-methyl group from the latter derivs. These results are rationalized in terms of the radical site formed on one unsatd. functional group attacking the polarizable  $\pi$ -electrons of the other unsatd. group. 24 references.  
IT 20637-11-0 20637-13-2  
RL: PRP (Properties)  
(mass spectrum of)  
RN 20637-11-0 CAPLUS  
CN (Phenyl sulfide)-2,2',4,4',6,6'-d<sub>6</sub> (8CI) (CA INDEX NAME)



RN 20637-13-2 CAPLUS  
CN (p-Tolyl sulfide)-2,2',6,6'-d<sub>4</sub> (8CI) (CA INDEX NAME)



=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

10/521,531

07/16/2008

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

252.14

430.71

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-36.80

-36.80

STN INTERNATIONAL LOGOFF AT 09:54:19 ON 16 JUL 2008